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MARTENSITIC PHASE TRANSITIONS
WITH SURFACE EFFECTS

by

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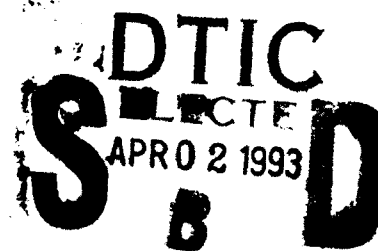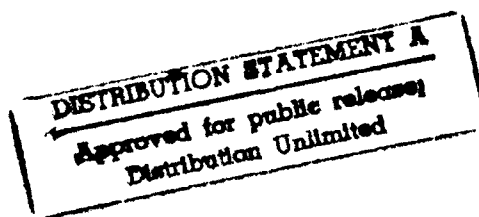
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Martensitic phase transitions with surface effects

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Abstract. A model of martensitic phase transitions is presented that is capable of accounting for a variety of surface effects associated with the localized interaction of coexisting phases of a material. Such phenomena are thought to play a critical role in determining the size, shape and stability of nucleated embryos as well as to affect the conditions under which nucleation occurs. Attention is restricted to transitions that are mechanically induced, and the model does not account for temperature effects. Materials that undergo martensitic phase changes are modeled as hyperelastic in both the bulk and the interface. The characterization of such bodies is examined in detail, and a representation theorem is presented for isotropic, hyperelastic interfaces in terms of two scalar invariants associated with the deformation of the interface.

1. Introduction

A subject of continuing interest in both the mechanics and materials science communities is non-diffusive phase transitions that involve two solid phases of a material separated by a sharp, coherent interface. These *martensitic* processes are most common in Fe-C systems, but are found in Ni-Ti, Ag-Cd, Au-Cd, Cu-Zn, Cu-Zn-Al, Cu-Al-Ni, In-Tl and other alloys as well [1–7]. In addition, some ceramic materials such as partially stabilized zirconia exhibit this type of phase transition [8–10].

In recent years the materials science community has developed a wide variety of products whose working properties rely on martensitic phase transitions. These include shape-memory materials like the Nitinol and Tinel alloys [11]. Another technology based on martensitic phase transitions is that of transformation-toughened materials [8–10].

Interest in martensitic materials has motivated a variety of theoretical investigations that help to better understand these phase transitions by modeling them from a continuum physics perspective [12–34]. Here *phases* refer to disjoint domains of a single energy functional that characterizes the material of interest.

This is in line with the intuitive picture that individual phases are just differing configurations of a single substance and provides a means of distinguishing the deformation of a given phase from a phase transition. The classical example of this type of material description is that for the Van der Waals fluid [35]. From the continuum point of view, an interface is coherent if the multiphase configuration can be described as a continuous deformation of some homogeneous reference state.

Material constitution generally imposes severe restrictions—*phase segregation requirements*—on the ways coherent coexistence can be accommodated. Multiphase states can be supported only under certain conditions, and the shape of each phase is often restricted as well [34]. The interface between phases may *accrete*—that is, move relative to the underlying material so as to effect a transfer of mass from one phase to another. However, it is not a free boundary because of the phase segregation requirements, and certain materials may call for supplementary information regarding interface position [21-23, 26, 29, 30].

Some continuum models do not capture certain key phenomena, known as *surface effects*, associated with phase transitions. These are due to the localized interaction of coexisting material phases. This interaction is particularly relevant in situations where the interface curvature is very large—as in the initial formation of a new phase embryo [41].

One such surface effect is the existence of a jump in the traction exerted on either side of an interface within a statics setting. In fluids, for example, the pressure inside a vapor bubble is higher than that of the surrounding liquid, but in solids it is reasonable to think that interfaces may resist shear as well, since this is a characteristic of the bulk phases on either side of the interface.

A second important effect attributable to interface properties is the occurrence of *supercritical phenomena* [36-40]. Conditions capable of initiating a phase change with planar interface geometry cannot produce a phase embryo with a highly curved boundary. For example, a phase change might not occur until

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the body is superheated above its normal transition temperature. Likewise, for mechanically induced reactions, a body may require straining beyond the level known to induce phase changes when inhomogeneities allow the formation of low curvature interfaces.

The symmetry properties associated with an interface influence the shape of a phase embryo, and this is especially true when the nucleus is so small that bulk effects do not dominate [41, 42]. The surface properties of an interface can thus play an important role in the determination of embryo shape.

A final surface effect pertains to the stability of newly formed nuclei which may depend upon the embryo size as well as on conditions at the system boundary. This behavior, and often the existence of such equilibria themselves, are attributable to localized properties at phase interfaces [38–40].

Continuum treatments of phase transitions may be modified to account for these important surface effects. Interface properties are modeled by fields defined on the interface itself, which are collectively referred to as *interfacial structure*. Here the interface is usually treated as a surface. Balance principles are postulated that restrict the way in which bulk and surface fields may interact, and materials are characterized by constitutive response functions. An historical survey of the evolution of such models is provided by LUSK [45].

For simplicity, attention is restricted to martensitic transitions that are mechanically induced, and the development presented here does not account for temperature effects. The theory is a modified version of that developed by GURTIN and STRUTHERS [46], and offers an alternate foundation for studying surface effects in martensitic phase transitions. Materials that undergo such changes are modeled as hyperelastic in both the bulk and the interface. The characterization of such bodies is examined in detail, and a representation theorem is presented for describing the interfaces of isotropic, hyperelastic bodies in terms of two fundamental scalar invariants associated with the deformation of the interface. An application of the theory is discussed in LUSK [47].

2. Preliminaries

Within a purely mechanical theory of phase transitions, phase interfaces are associated with strain discontinuities. For clarity of presentation, the theory presented here assumes there exists at most one such interface in a given body.

2.1 Notation and definitions

$\mathbb{R}^N$	set of all N-tuples of real numbers
$\mathcal{V}^N, \mathcal{U}^N$	N-dimensional inner product spaces
$\mathbb{E}^N$	N-dimensional Euclidean space
$\mathrm{Unit}(\mathcal{V}^N)$	set of all unit length elements of $\mathcal{V}^N$
$\mathrm{Lin}(\mathcal{V}^N, \mathcal{V}^M)$	set of all linear maps of $\mathcal{V}^N \to \mathcal{V}^M$
$\mathrm{Lin}^{NS}(\mathcal{V}^N, \mathcal{V}^M)$	set of all non-singular elements of $\mathrm{Lin}(\mathcal{V}^N, \mathcal{V}^M)$
$\mathrm{Lin}_+(\mathcal{V}^N, \mathcal{U}^N)$	set of all elements of $\mathrm{Lin}(\mathcal{V}^N, \mathcal{U}^N)$ with positive determinant
$\mathrm{Sym}(\mathcal{V}^N)$	set of all symmetric elements of $\mathrm{Lin}(\mathcal{V}^N, \mathcal{V}^N)$
$\mathrm{Sym}^+(\mathcal{V}^N)$	set of all positive definite elements of $\mathrm{Sym}(\mathcal{V}^N)$
$\mathrm{Unim}(\mathcal{V}^N, \mathcal{U}^N)$	set of all elements of $\mathrm{Lin}_+(\mathcal{V}^N, \mathcal{U}^N)$ with unit determinant
$\mathrm{Orth}(\mathcal{V}^N, \mathcal{U}^N)$	set of all orthogonal elements of $\mathrm{Lin}(\mathcal{V}^N, \mathcal{U}^N)$
$\mathrm{Orth}_+(\mathcal{V}^N, \mathcal{U}^N)$	set of all orthogonal elements of $\mathrm{Lin}_+(\mathcal{V}^N, \mathcal{U}^N)$

The *inner product* of $\mathbf{a}, \mathbf{b} \in \mathcal{V}^N$ is denoted by $< \mathbf{a}, \mathbf{b} >$ or $\mathbf{a} \cdot \mathbf{b}$. The *outer product* of $\mathbf{c} \in \mathcal{V}^N$ and $\mathbf{d} \in \mathcal{V}^M$ is denoted by $\mathbf{c} \otimes \mathbf{d} \in \mathrm{Lin}(\mathcal{V}^N, \mathcal{V}^M)$. The *vector product* of $\mathbf{f}, \mathbf{g} \in \mathcal{V}^N$ is denoted by $(\mathbf{f} \wedge \mathbf{g}) \in \mathcal{V}^N$. The *inner product* on $\mathrm{Lin}(\mathcal{V}^N, \mathcal{V}^M)$ is defined by

$$\mathbf{A} \cdot \mathbf{B} := \mathrm{Trace}(\mathbf{A}\mathbf{B}^T) = \langle \mathbf{A}, \mathbf{B} \rangle \quad \forall \mathbf{A}, \mathbf{B} \in \mathrm{Lin}(\mathcal{V}^N, \mathcal{V}^M) \qquad (2.1)$$

so that all of the sets of linear transformations defined above are endowed with an inner product space structure.

In general, scalar fields are denoted by lower-case letters, vector fields by lower-case bold type, and tensor fields by bold-type, upper-case letters. A super-

script '·' denotes partial differentiation with respect to the second argument of a function.

Surface S	a subset of $I\!\!E^3$ locally diffeomorphic to $I\!\!E^2$.
Surface normal $n(x)$	either of the two unit vectors perpendicular to a surface at the point x.
Tangent space $n^\perp(x)$ of S at x	best linear approximation to S at x.
Surface boundary ∂S	the closed curve that delineates the edge of a surface.
Tangential vector field	field on S with values in $n^\perp(x)$.
Tangential tensor field	field on S with values in $\mathrm{Lin}(n^\perp(x), n^\perp(x))$.
Boundary bi-normal, $m(x)$	the outward pointing unit vector perpendicular to ∂S at x but within the tangent space of S at that point.
Projection map P of S	tensor field on S with values in $\mathrm{Lin}(I\!\!E^3, n^\perp(x))$ defined by $P(x)a = a - (a \cdot n(x))n(x)$ $\forall x \in S, \forall a \in I\!\!E^3$.
Inclusion map I of S	tensor field on S with values in $\mathrm{Lin}(n^\perp(x), I\!\!E^3)$ defined by $I(x)a = a \quad \forall x \in S, \quad \forall a \in n^\perp(x)$. $P(x)I(x) = 1_s$, the tangent space identity map at x, while $I(x)P(x) = 1 - n(x) \otimes n(x)$. Also, $I = P^T$.

2.2 Bulk and surface gradients

Let $g : I\!\!E^K \to I\!\!E^N$. Then for every x in $I\!\!E^K$ the gradient of g at x, denoted by $\nabla g(x)$, is the unique element of $\mathrm{Lin}(I\!\!E^K, I\!\!E^N)$ such that

$$\lim_{h \searrow 0} \left(g(x + hk) - (\nabla g(x))hk \right) = g(x) \quad \forall k \in I\!\!E^K. \tag{2.2}$$

Now consider a scalar field g defined on S instead of $I\!\!E^K$. Let ϕ *parameterize* S—that is $\phi : I\!\!E^2 \to S$ diffeomorphically. Then there exists $f : I\!\!E^2 \to I\!\!R$ given by

the composition $f := g \circ \phi$ which allows the gradient of g to be defined as

$$\nabla g(\mathbf{x}) := (\nabla f) \circ (\nabla \phi)^{-1}. \tag{2.3}$$

It is straightforward to show that this definition of the gradient of a scalar field is independent of the parameterization ϕ of S. The idea is extendable to vector and tensor fields on S as well. For emphasis, denote by ∇_s the *surface* gradient of a field on S. Note that if w, $\mathbf{b}$, and $\mathbf{A}$ are scalar, vector, and tensor fields on S, respectively, then

$$\nabla_s w(\mathbf{x}) \in \mathbf{n}^\perp(\mathbf{x})$$
$$\nabla_s \mathbf{b}(\mathbf{x}) \in \mathrm{Lin}\big(\mathbf{n}^\perp(\mathbf{x}), E^3\big) \tag{2.4}$$
$$\nabla_s \mathbf{A}(\mathbf{x}) \in \mathrm{Lin}\big(\mathbf{n}^\perp(\mathbf{x}), \mathrm{Lin}(E^3, E^3)\big).$$

2.3 Smooth fields and surface divergence

Let $w : S \to I\!\!R$ be a map such that $\nabla_s w$ is defined on S. Then w is *smooth* on S and is this is denoted by $w \in C^1(S)$ or sometimes by $w : S \xrightarrow{c^1} I\!\!R$. The extension to vector and tensor fields is completely analogous. If $\hat{\mathbf{b}}$ is a smooth, vector field on S then $\nabla_s \cdot \hat{\mathbf{b}} := \mathrm{Trace}\big(\mathbf{P}\nabla_s \hat{\mathbf{b}}\big)$ on S is the *surface divergence* of $\hat{\mathbf{b}}$. Analogously, for $\hat{\mathbf{C}}$ a smooth, tensor field on S the surface divergence of $\hat{\mathbf{C}}$ is given by

$$(\nabla_s \cdot \hat{\mathbf{C}}) \cdot \mathbf{k} = \nabla_s \cdot (\hat{\mathbf{C}}^T k) \quad \forall \mathbf{k} \in E^3. \tag{2.5}$$

The tangential tensor field $\mathbf{L} := -\mathbf{P}\nabla_s \mathbf{n}$ provides curvature information intrinsic to the surface and is therefore called the *curvature tensor*. It can be shown that $\mathbf{L}$ is symmetric and that the scalar field $H := \frac{1}{2}\mathrm{Trace}(\mathbf{L})$ gives the surface *mean curvature*. A corollary to the Stokes theorem that is useful for surface considerations is the

SURFACE DIVERGENCE THEOREM.

Let $\mathbf{f}$ be a smooth, vector field on S. Then

$$\int_S \nabla_s \cdot \mathbf{f} \, dA = \int_{\partial S} \mathbf{f} \cdot \mathbf{m} \, dL - \int_S 2H(\mathbf{f} \cdot \mathbf{n}) \, dA. \tag{2.6}$$

2.4 Surface motion

Consider a one-parameter family of surfaces $S(t)$ defined over some open time interval T. Let

$$S_T := \{(\mathbf{x}, t) | \mathbf{x} \in S(t), \quad t \in T\}$$

$$(\partial S)_T := \{(\mathbf{x}, t) | \mathbf{x} \in \partial S(t), \quad t \in T\} \tag{2.7}$$

define the *surface* and *surface-boundary trajectories*. Let $\phi : U \subset E^2 \times T \to S_T$ be a one-parameter family of surface parameterizations. Denote by ϕ_∂ the restriction of ϕ to $\partial U \times T$, where ∂U is the boundary of U. If there exists a ϕ such that $\dot\phi$ is defined on $U \times T$ and $\dot\phi_\partial$ is defined on $\partial U \times T$, then the surface is said to be *smoothly propagating*. It can be shown that while the *interface* and *edge velocities*

$$\mathbf{V}(\mathbf{x}, t) := \dot\phi(\phi^{-1}(\mathbf{x}, t), t)$$

$$\mathbf{V}_\partial(\mathbf{x}, t) := \dot\phi_\partial(\phi^{-1}(\mathbf{x}, t), t) \tag{2.8}$$

depend on the choice of parameterization ϕ the *normal* and *intrinsic edge speeds*,

$$V_n := \mathbf{V} \cdot \mathbf{n} \quad \text{on} \quad S_T$$

$$V_m := \mathbf{V} \cdot \mathbf{m} \quad \text{on} \quad \partial S_T, \tag{2.9}$$

are independent of parameterization. $V_n \mathbf{n}$ is the *normal velocity* of S. $V_m \mathbf{m}$ is the *intrinsic, tangential edge velocity* of S. On the surface boundary, the sum of these two velocity fields is referred to as the *intrinsic edge velocity* of S.

Consider a *normal trajectory* of S_T through $\mathbf{x} \in S(t_0)$, $t_0 \in T$. This is a smooth, t-parameterized curve in E^3 described by a set of position vectors $\mathbf{z}$ such that

$$\mathbf{z}(t) \in S(t), \quad \mathbf{P}(\mathbf{z}(t))\dot{\mathbf{z}}(t) = 0, \quad \forall t \in T. \tag{2.10}$$

The normal trajectory is used to define a *time derivative following S* by

$$\mathring{g}(\mathbf{x}, t) := \frac{d}{dt} g(\mathbf{z}(t), t), \tag{2.11}$$

where $\mathbf{z}$ gives the normal trajectory of S_T through $\mathbf{x} \in S(t)$. It may be shown that

$$\mathring{\mathbf{n}} = -\nabla_s V_n. \tag{2.12}$$

This derivative also finds application in the

SURFACE TRANSPORT THEOREM.

Let g be a smooth scalar field on a smoothly propagating surface $\mathcal{S}$. Then

$$\frac{d}{dt} \int_{\mathcal{S}(t)} g \, dA = \int_{\mathcal{S}(t)} \left[\overset{\circ}{g} - 2HgV_n \right] dA + \int_{\partial\mathcal{S}(t)} gV_m \, dL \quad \forall t \in \mathcal{T}. \tag{2.13}$$

2.5 Latticed bodies and interfaces

A collection $\mathcal{B}$ of elements p is a *body* if there is a set $\Omega(\mathcal{B})$ of continuous bijections $\mathcal{X}$ such that:

(i)   the gradient of the induced map between any two elements has positive determinant where it is defined;

(ii) $\Omega(\mathcal{B})$ contains all continuous bijections of its elements.

A *lattice* $\mathcal{L}(\mathcal{B})$ of a body $\mathcal{B}$ is a set of elements of $\Omega(\mathcal{B})$ such that:

(i)   the gradient of the induced map between any two elements is smooth;

(ii) $\mathcal{L}(\mathcal{B})$ contains all smooth bijections (diffeomorphisms) of its elements.

A *latticed body* is any body together with one of its lattices. The view is taken that a body must be provided with a lattice—a preferred group of reference configurations—in order to identify phase interfaces kinematically.

A *two-phase deformation* with respect to $\mathcal{K} \in \Omega(\mathcal{B})$ is a configuration $\mathcal{X} \in \Omega(\mathcal{B})$ such that the induced map between $\mathcal{K}$ and $\mathcal{X}$ is arbitrarily smooth everywhere except possibly on a *phase interface S*. A *two-phase motion* $\mathcal{X}_{\mathcal{T}}$ is a one-parameter family of two-phase deformations $\mathcal{X}(t) \in \Omega(\mathcal{B})$ with t ranging over an open interval $\mathcal{T}$. It is *admissible* if there exists a reference configuration $\mathcal{K} \in \Omega(\mathcal{B})$ such that

(i)   each element of $\mathcal{X}_{\mathcal{T}}$ is a two-phase deformation with respect to $\mathcal{K}$;

(ii) $\mathcal{S}_{\mathcal{T}}$ is a smoothly propagating surface.

For a latticed body to undergo an admissible, two-phase deformation it must be admissible with respect to one, and hence all, of the elements of its lattice.

Consider the two-phase deformation shown in Fig. 1 with induced map $\bar{y}$ and bulk deformation gradient $\mathbf{F} := \nabla \bar{y}$ defined where $\bar{y}$ is smooth. Then the surface in the deformed configuration of the body,

$$\bar{S} := \left\{ \mathbf{y} \,\middle|\, \mathbf{y} = \bar{y}(\mathbf{x}), \quad \mathbf{x} \in S \right\}, \tag{2.14}$$

is referred to as the *deformed interface* with $\{\bar{n}, \bar{m}\}$ and $\bar{\mathbf{P}}$ its surface orientations and projection map. The restriction of $\bar{y}$ to S, denoted by $\hat{y}$, is the invertible deformation map of the surface with an associated *surface deformation gradient* $\hat{\mathbf{F}} := \nabla_s \hat{y}$ defined on S. Note that $\hat{\mathbf{F}}(\mathbf{x}) \in \mathrm{Lin}_+(\mathbf{n}^\perp(\mathbf{x}), \bar{n}^\perp(\mathbf{y}))$, $\mathbf{y} = \hat{y}(\mathbf{x})$, even though $\mathbf{F}$ is not defined on S. It is often convenient to use the linear transformation representing the surface gradient of $\bar{y}$:

$$\mathbb{F} := \nabla_s \bar{y} = \mathbf{F}^+ \mathbf{I} = \mathbf{F}^- \mathbf{I}, \tag{2.15}$$

where

$$\mathbf{F}^{\pm} = \lim_{l \searrow 0} \left[\mathbf{F}\left(\mathbf{x} \pm l\mathbf{n}(\mathbf{x})\right) \right] \quad \forall \mathbf{x} \in S. \tag{2.16}$$

Thus,

$$\hat{\mathbf{F}} = \bar{\mathbf{P}}\mathbb{F}, \quad \mathbf{F}^{\pm} = \mathbb{F}\mathbf{P} + \left(\mathbf{F}^{\pm}\right)\mathbf{n} \otimes \mathbf{n}, \tag{2.17}$$

and it is easy to show that

$$\mathbb{F} = \bar{\mathbf{I}}\hat{\mathbf{F}}. \tag{2.18}$$

Note that $\mathbb{F} \in \mathrm{Lin}^{NS}(\mathbf{n}^\perp, \mathbb{E}^3)$.

The orientations of the undeformed and deformed interfaces may be related using the determinants of the deformation gradients

$$\begin{aligned} J &:= \mathrm{Det}(\mathbf{F}) \\ j &:= \mathrm{Det}(\hat{\mathbf{F}}) = \frac{\mathrm{Det}(\mathbf{F})}{\|\mathbf{F}^{-T}\mathbf{n}\|} \end{aligned} \tag{2.19}$$

where $\mathbf{F}$ may be either $\mathbf{F}^+$ or $\mathbf{F}^-$ in the second equality. The relations are

$$\bar{n} = \frac{J}{j}\mathbf{F}^{-T}\mathbf{n}, \quad \bar{m} = \frac{j}{h}\hat{\mathbf{F}}^{-T}\mathbf{m}, \tag{2.20}$$

where $\mathbf{F}$ may be either $\mathbf{F}^+$ or $\mathbf{F}^-$ and where h is the determinant of the gradient of the restriction of $\bar{\mathbf{y}}$ to $\partial \mathcal{S}$.

Define the *material* and *spatial velocity fields*, $\mathbf{v}$ and $\bar{\mathbf{v}}$ respectively, as

$$\mathbf{v}(\mathbf{x}, t) := \dot{\mathbf{y}}(\mathbf{x}, t)$$
$$\bar{\mathbf{v}}(\mathbf{y}, t) := \mathbf{v}(\bar{\mathbf{y}}^{-1}(\mathbf{y}, t), t). \tag{2.21}$$

If $\mathbf{V}$ is a surface velocity of $\mathcal{S}_T$, then the *induced interface velocity*

$$\bar{\mathbf{V}} := (\mathbf{F} \underset{\pm}{}) \mathbf{V} + \mathbf{v}^{\pm} \tag{2.22}$$

is a surface velocity for $\bar{\mathcal{S}}_T$—the interface trajectory associated with deforming interface $\mathcal{S}$. As (2.22) indicates, the definition of $\bar{\mathbf{V}}$ does not depend on the side of $\bar{\mathcal{S}}$ used and in fact

$$\bar{\mathbf{V}} = \mathbf{F}_c \mathbf{V} + \mathbf{v}_c \quad \forall c \in [0, 1] \tag{2.23}$$

where

$$\mathbf{F}_c := c\mathbf{F}^+ + (1 - c)\mathbf{F}^-$$
$$\mathbf{v}_c := c\mathbf{v}^+ + (1 - c)\mathbf{v}^-. \tag{2.24}$$

Let $\mathcal{K}_1$ and $\mathcal{K}_2$ be lattice elements related by the linear transformation $\mathbf{G}$: $\mathcal{K}_1(\mathcal{B}) \to \mathcal{K}_2(\mathcal{B})$. If $\mathbf{V}_1$ is an interface velocity for the motion with respect to $\mathcal{K}_1$, then $\mathbf{V}_2 = \mathbf{G}\mathbf{V}_1$ is an interface velocity for the motion with respect to $\mathcal{K}_2$ with $\mathbf{V}_1$ and $\mathbf{V}_2$ inducing the same interface trajectory $\bar{\mathcal{S}}_T$.

2.6 Galilean objectivity

Consider the admissible, two-phase motions $\mathcal{X}_T$ and $\mathcal{X}_T^*$ of a latticed body $\{\mathcal{B}, \mathcal{L}\}$ with

$$\mathcal{X}^*(t) = \mathbf{Q}\mathcal{X}(t) + \mathbf{d}t + \mathbf{e} \quad \forall t \in \mathcal{T},$$

and

$$\mathbf{Q} \in \text{Orth}_+(\mathbb{E}^3, \mathbb{E}^3), \qquad \mathbf{d}, \mathbf{e} \in \mathbb{E}^3.$$

Denote by $\bar{\mathcal{R}}(t) := \mathcal{X}(t; \mathcal{B})$ the region occupied by $\mathcal{B}$ for all t in $\mathcal{T}$, with $\bar{\mathcal{S}}_{\mathcal{T}}$ the deformed interface trajectory partitioning $\bar{\mathcal{R}}(t)$ over $\mathcal{T}$. Define the *bulk trajectory* as

$$\bar{\mathcal{R}}_{\mathcal{T}} := \left\{ (\mathbf{y}, t) \big| \, \mathbf{y} \in \bar{\mathcal{R}}(t), \quad t \in \mathcal{T} \right\}.$$

Suppose that

$$\phi : \quad (\bar{\mathcal{R}}_{\mathcal{T}} \setminus \bar{\mathcal{S}}_{\mathcal{T}}) \to \mathbb{R}$$

$$\mathbf{A} : \quad (\bar{\mathcal{R}}_{\mathcal{T}} \setminus \bar{\mathcal{S}}_{\mathcal{T}}) \to \mathrm{Lin}(\mathbb{E}^3, \mathbb{E}^3)$$

$$\hat{\phi} : \quad \bar{\mathcal{S}}_{\mathcal{T}} \to \mathbb{R}$$

$$\hat{\mathbf{A}} : \quad (\mathbf{y}, t) \in \bar{\mathcal{S}}_{\mathcal{T}} \mapsto \hat{\mathbf{A}}(\mathbf{y}, t) \in \mathrm{Lin}\big(\bar{\mathbf{n}}^{\perp}(\mathbf{y}, t), \mathbb{E}^3 \big)$$

are fields associated with $\{\mathcal{B}, \mathcal{L}\}$ during motion $\mathcal{X}_{\mathcal{T}}$ and that

$$\phi^* : \quad (\bar{\mathcal{R}}_{\mathcal{T}}^* \setminus \bar{\mathcal{S}}_{\mathcal{T}}^*) \to \mathbb{R}$$

$$\mathbf{A}^* : \quad (\bar{\mathcal{R}}_{\mathcal{T}}^* \setminus \bar{\mathcal{S}}_{\mathcal{T}}^*) \to \mathrm{Lin}(\mathbb{E}^3, \mathbb{E}^3)$$

$$\hat{\phi}^* : \quad \bar{\mathcal{S}}_{\mathcal{T}}^* \to \mathbb{R}$$

$$\hat{\mathbf{A}}^* : \quad (\mathbf{y}, t) \in \bar{\mathcal{S}}_{\mathcal{T}}^* \mapsto \hat{\mathbf{A}}^*(\mathbf{y}, t) \in \mathrm{Lin}\big(\bar{\mathbf{n}}^{\perp}(\mathbf{y}, t), \mathbb{E}^3 \big)$$

are the analogous fields of $\{\mathcal{B}, \mathcal{L}\}$ during motion $\mathcal{X}_{\mathcal{T}}^*$. The fields associated with $\{\mathcal{B}, \mathcal{L}\}$ are said to exhibit *Galilean objectivity* if

$$\phi^*\big(\mathbf{z}^*(\mathbf{y}, t), t\big) = \phi(\mathbf{y}, t)$$
$$\mathbf{A}^*\big(\mathbf{z}^*(\mathbf{y}, t), t\big) = \mathbf{Q}\mathbf{A}(\mathbf{y}, t)\mathbf{Q}^T \qquad \forall (\mathbf{y}, t) \in \bar{\mathcal{R}}_{\mathcal{T}} \setminus \bar{\mathcal{S}}_{\mathcal{T}}$$

and

$$\hat{\phi}^*\big(\mathbf{z}^*(\mathbf{y}, t), t\big) = \hat{\phi}(\mathbf{y}, t)$$
$$\hat{\mathbf{A}}^*\big(\mathbf{z}^*(\mathbf{y}, t), t\big) = \mathbf{Q}\hat{\mathbf{A}}(\mathbf{y}, t)\mathbf{Q}^T \qquad \forall (\mathbf{y}, t) \in \bar{\mathcal{S}}_{\mathcal{T}},$$

where

$$\mathbf{z}^*(\mathbf{y}, t) := \mathbf{Q}\mathbf{y} + \mathbf{d}t + \mathbf{e} \quad \forall (\mathbf{y}, t) \in \bar{\mathcal{R}}_{\mathcal{T}}.$$

3. Balance postulates

3.1 Primitive fields

Consider a latticed body $\{\mathcal{B}, \mathcal{L}\}$ and an admissible two-phase motion $\mathcal{X}_\tau$, and let $\bar{\mathcal{R}}_\tau$ and $\bar{\mathcal{S}}_\tau$ be the bulk and interface trajectories discussed in section 2.6. Stipulate that for every such motion the following smooth fields exist:

Bulk mass density	$\bar{\rho}:$	$(\mathcal{R}_\tau \setminus \hat{\mathcal{S}}_\tau) \to I\!\!R_+$
Bulk energy density	$W:$	$(\mathcal{R}_\tau \setminus \hat{\mathcal{S}}_\tau) \to I\!\!R$
Cauchy stress	$T:$	$(\bar{\mathcal{R}}_\tau \setminus \hat{\mathcal{S}}_\tau) \to \mathrm{Lin}(I\!\!E^3, I\!\!E^3)$
Interfacial energy density	$\bar{w}:$	$\hat{\mathcal{S}}_\tau \to I\!\!R$
Deformational surface stress	$\hat{\mathbf{T}}:$	$(y,t) \in \bar{\mathcal{S}}_\tau \mapsto \hat{\mathbf{T}}(y,t) \in \mathrm{Lin}\big(\bar{\mathbf{n}}^\perp(y,t), I\!\!E^3\big)$
Accretive surface stress	$\hat{\mathbf{C}}:$	$(y,t) \in \bar{\mathcal{S}}_\tau \mapsto \hat{\mathbf{T}}(y,t) \in \mathrm{Lin}\big(\bar{\mathbf{n}}^\perp(y,t), I\!\!E^3\big)$

3.2 Balance postulates

Let $\bar{\mathcal{P}}_\tau$ be the bulk trajectory associated with an arbitrary subbody of $\mathcal{B}$ under the previous motion $\mathcal{X}_\tau$ as shown in Fig. 2. Denote by $\bar{\mathcal{Q}}_\tau$ the partitioning subinterface trajectory associated with $\bar{\mathcal{P}}_\tau$. The boundary of $\bar{\mathcal{Q}}$ is denoted by $\partial\bar{\mathcal{Q}}$. Let $\bar{\nu}$ be the outward unit normal to $\partial\bar{\mathcal{P}}$—the boundary of $\bar{\mathcal{P}}$. Interface normal $\bar{\mathbf{n}}$ and bi-normal $\bar{\mathbf{m}}$ are as defined in section 2. The following postulates are imposed on all such subregions and motions. The theory presented here is a modified version of that developed by GURTIN and STRUTHERS ['6].

MASS CONSERVATION

$$\frac{d}{dt} \int\limits_{\bar{\mathcal{P}}(t)} \bar{\rho}\, dV = 0$$

Momenta Balances

$$\frac{d}{dt} \int_{\bar{\mathcal{P}}(t)} \bar{\rho}\mathbf{v}\, dV = \int_{\partial\bar{\mathcal{P}}(t)} \mathbf{T}\bar{\nu}\, dA + \int_{\partial\bar{\mathcal{Q}}(t)} \hat{\mathbf{T}}\bar{m}\, dL$$

$$\frac{d}{dt} \int_{\bar{\mathcal{P}}(t)} \mathbf{y}\wedge\bar{\rho}\mathbf{v}\, dV = \int_{\partial\bar{\mathcal{P}}(t)} \mathbf{y}\wedge\mathbf{T}\bar{\nu}\, dA + \int_{\partial\bar{\mathcal{Q}}(t)} \mathbf{y}\wedge\hat{\mathbf{T}}\bar{m}\, dL$$

Mechanical Dissipation Imbalance

$$\dot{E} + \dot{K} \le P,$$

where

$$E\left(t;\bar{\mathcal{P}}(t)\right) := \int_{\bar{\mathcal{P}}(t)} \bar{W}\, dV + \int_{\bar{\mathcal{Q}}(t)} \bar{w}\, dA$$

$$K\left(t;\bar{\mathcal{P}}(t)\right) := \int_{\bar{\mathcal{P}}(t)} \frac{1}{2}\bar{\rho}\bar{\mathbf{v}}\cdot\mathbf{v}\, dV$$

$$P\left(t;\bar{\mathcal{P}}(t)\right) := \int_{\partial\bar{\mathcal{P}}(t)} \mathbf{T}\bar{\nu}\cdot\mathbf{v}\, dA + \int_{\partial\bar{\mathcal{Q}}(t)} \hat{\mathbf{T}}\bar{m}\cdot\bar{\mathbf{V}}\, dL + \int_{\partial\bar{\mathcal{Q}}(t)} \hat{\bar{\mathbf{C}}}\bar{m}\cdot\left(\bar{\mathbf{V}} - \bar{\mathbf{v}}^{+}\right)\, dL$$

$$+ \int_{\partial\bar{\mathcal{Q}}(t)} \hat{\bar{\mathbf{C}}}\bar{m}\cdot\left(\bar{\mathbf{V}} - \bar{\mathbf{v}}^{-}\right)\, dL.$$

Parameterization Invariance

The power P expended at the boundary of $\bar{\mathcal{P}}$ is independent of the parameterization of $\bar{\mathcal{Q}}$ for all times in $\mathcal{T}$.

Objectivity

$\bar{W}$, $\bar{w}$, $\mathbf{T}$, $\hat{\mathbf{T}}$, and $\hat{\bar{\mathbf{C}}}$ exhibit Galilean objectivity as defined in section 2.

By Cauchy's theorem, the momenta balances imply that $\mathbf{T}$ is symmetric. A curvilinear triangle version of the theorem applied on the interface shows that the deformational surface stress $\hat{\mathbf{T}}$ is symmetric as well, and is therefore representable

as a tangential tensor field as defined in section 2.1. Henceforth $\hat{\mathbf{T}}$ is taken to be tangential. Note that symmetry of $\mathbf{T}$ and $\hat{\mathbf{T}}$ together with conservation of linear momentum implies the angular momentum balance.

The presence of two distinct interfacial stresses taxes physical intuition, and this issue is addressed at several points in the ensuing development. The deformational stress $\hat{\mathbf{T}}$ expends power in association with the *absolute* movement of the interface. Even during a two-phase motion for which no new material changes phase, work is performed by this stress. In contrast, the accretive stress $\overset{\approx}{\mathbf{C}}$ expends power in association with the *relative* motion of the interface with respect to the underlying material—a process referred to as *accretion*. In the limiting case, not covered by this theory, of a phase transition occurring with *no* material deformation the accretive stress may still expend power. This stress is the Eulerian counterpart to that presented by GURTIN and STRUTHERS [46] and is related to the capillary tractions of LEO and SEKERKA [48], CAHN and HOFFMAN [49] and HOFFMAN and CAHN [50]. Its physical significance for *hyperelastic* materials is elucidated in sections 4 and 5.

3.3 Referential formulation

The derivation of local field equations is facilitated by re-expressing all primitive fields as quantities defined on an arbitrary element of the body lattice, as shown in Fig. 2. To this end, define the following fields on such a reference configuration:

Referential mass density	$\rho := J\bar{\rho}$
Referential bulk energy	$W := J\bar{W}$
Piola-Kirchhoff stress	$\mathbf{S} := J\mathbf{TF}^{-T}$
Referential interfacial energy	$w := j\bar{w}$
Referential deformational surface Stress	$\hat{\mathbf{S}} := j\bar{\mathbf{I}}\hat{\mathbf{T}}\hat{\mathbf{F}}^{-T}, \quad j\hat{\mathbf{T}} = \bar{\mathbf{P}}\hat{\mathbf{S}}\hat{\mathbf{F}}^{T}$
Referential accretive surface stress	$\hat{\mathbf{C}} := 2j\langle\!\langle\mathbf{F}^{T}\rangle\!\rangle\overset{\approx}{\mathbf{C}}\hat{\mathbf{F}}^{-T},$

where $\mathbf{F}$, $\hat{\mathbf{F}}$, j, and J are as defined in section 2.5 and

$$\langle\!\langle \phi(\mathbf{x}) \rangle\!\rangle := \lim_{h \searrow 0} \frac{1}{2} \big\{ \phi(\mathbf{x} + h\mathbf{n}(\mathbf{x})) + \phi(\mathbf{x} - h\mathbf{n}(\mathbf{x})) \big\} \quad \forall \mathbf{x} \in \mathcal{S}. \qquad (3.1)$$

Using these fields, the linear momentum balance and the mechanical dissipation imbalance can be expressed as

$$\frac{d}{dt} \int_{\mathcal{P}} \rho \mathbf{v} \, dV = \int_{\partial \mathcal{P}} \mathbf{S}\nu \, dA + \int_{\partial \mathcal{Q}(t)} \hat{\mathbf{S}}\mathbf{m} \, dL \qquad (3.2)$$

and

$$\frac{d}{dt} \int_{\mathcal{P}} W \, dV + \frac{d}{dt} \int_{\mathcal{Q}(t)} w \, dA + \frac{d}{dt} \int_{\mathcal{P}} \frac{1}{2} \rho \mathbf{v} \cdot \mathbf{v} \, dV$$
$$\leq \int_{\partial \mathcal{P}} \mathbf{S}\nu \cdot \mathbf{v} \, dA + \int_{\partial \mathcal{Q}(t)} \hat{\mathbf{S}}\mathbf{m} \cdot \big[\mathbf{F}_c \mathbf{V} + \mathbf{v}_c \big] \, dL + \int_{\partial \mathcal{Q}(t)} \hat{\mathbf{C}}\mathbf{m} \cdot \mathbf{V} \, dL, \qquad (3.3)$$

with $\mathbf{F}_c$ and $\mathbf{v}_c$ defined by (2.24).

The respective localizations of the linear momentum balance away from and local to the interface are

$$\nabla \cdot \mathbf{S} = \rho \mathbf{v}$$
$$[\![\rho \mathbf{v}]\!] V_n + [\![\mathbf{Sn}]\!] = -\nabla_s \cdot \hat{\mathbf{S}}. \qquad (3.4)$$

Here

$$[\![\phi(\mathbf{x})]\!] := \lim_{h \searrow 0} \big\{ \phi(\mathbf{x} + h\mathbf{n}(\mathbf{x})) - \phi(\mathbf{x} - h\mathbf{n}(\mathbf{x})) \big\} \quad \forall \mathbf{x} \in \mathcal{S}. \qquad (3.5)$$

Analogous localizations for the dissipation imbalance are made after considering the field restrictions imposed by the principle of parameterization invariance.

3.4 Implications of parameterization invariance

Use of the surface divergence theorem gives

$$\int_{\partial \mathcal{Q}(t)} \hat{\mathbf{C}}\mathbf{m} \cdot \mathbf{V} \, dL = \int_{\mathcal{Q}(t)} \nabla_s \cdot (\hat{\mathbf{C}}^T \mathbf{m} \cdot V_m \mathbf{m}) dA, \qquad (3.6)$$

and application of the product rule then yields

$$\int\limits_{\partial \mathcal{Q}(t)} \hat{\mathbf{C}}\mathbf{m}\cdot\mathbf{V}\,dL = \int\limits_{\mathcal{Q}(t)} \left[-\hat{\mathbf{C}}\cdot\mathbf{L}V_n - \hat{\mathbf{C}}^T\mathbf{n}\cdot\mathring{\mathbf{n}} + (\nabla_s\cdot\hat{\mathbf{C}})\cdot\mathbf{n}V_n\right]dA + \int\limits_{\partial \mathcal{Q}(t)} \hat{\mathbf{C}}\mathbf{m}\cdot\mathbf{m}V_m\,dL.$$

$$(3.7)$$

Now consider the second term in the referential dissipation inequality,

$$\int\limits_{\partial \mathcal{Q}(t)} \hat{\mathbf{S}}\mathbf{m}\cdot\left[\mathbf{F}_c\mathbf{V} + \mathbf{v}_c\right]dL. \qquad (3.8)$$

By the surface divergence theorem this is equal to

$$\int\limits_{\mathcal{Q}(t)} \nabla_s\cdot\left[\hat{\mathbf{S}}^T\mathbf{F}_c\mathbf{n}V_n\right]dA + \int\limits_{\mathcal{Q}(t)} \nabla_s\cdot\left[\hat{\mathbf{S}}^T\mathbf{v}_c\right]dA + \int\limits_{\partial \mathcal{Q}(t)} \hat{\mathbf{S}}\mathbf{m}\cdot\left[\mathbf{F}_c\mathbf{m}V_m\right]dL$$

$$= \int\limits_{\partial \mathcal{Q}(t)} \hat{\mathbf{S}}\mathbf{m}\cdot(\mathbf{F}_c\mathbf{m})V_m\,dL - \int\limits_{\mathcal{Q}(t)} \left[(\mathbb{F}\hat{\mathbf{S}})\cdot\mathbf{L} + (\nabla_s\cdot\hat{\mathbf{S}})\cdot(\mathbf{F}_c\mathbf{n})\right]V_n\,dA \qquad (3.9)$$

$$+ \int\limits_{\mathcal{Q}(t)} \left\{(\hat{\mathbf{S}}\mathbf{P})\cdot\mathring{\mathbf{F}}_c - (\hat{\mathbf{S}}^T\mathbf{F}_c\mathbf{n})\cdot\mathring{\mathbf{n}} + (\nabla_s\cdot\hat{\mathbf{S}})\cdot\mathbf{v}_c\right\}dA.$$

The mechanical dissipation imbalance is now expressible in a form amenable to application of the

INVARIANCE LEMMA. Let

$$e: \quad (\mathcal{R}_\tau \setminus \mathcal{S}_\tau) \to \mathbb{R}$$

$$f: \quad \mathcal{S}_\tau \to \mathbb{R}$$

$$g: \quad \mathcal{S}_\tau \to \mathbb{R},$$

and suppose that

$$\int\limits_{\mathcal{P}} e\,dV + \int\limits_{\mathcal{Q}(t)} f\,dA + \int\limits_{\partial \mathcal{Q}(t)} gV_m\,dL \le 0 \quad \forall \mathcal{P} \subset \mathcal{R}, \quad \forall t \in \mathcal{T}.$$

Then $g = 0$ on $\mathcal{S}_\tau$.

This is proved in [46]. The result restricts the primitive fields by the parameterization invariance postulate, which comes in the form of the

TENSION-ENERGY THEOREM [46].

$$\mathbb{F}^T \hat{\mathbf{S}} + \mathbf{P}\hat{\mathbf{C}} = w\mathbf{1}_s. \tag{3.10}$$

Equations (3.3) and (3.7)–(3.10) then combine to give a form of the mechanical dissipation imbalance that is consistent with the parameterization invariance postulate:

$$\frac{d}{dt}\int_{\mathcal{P}} W\,dV + \frac{d}{dt}\int_{\partial\mathcal{Q}(t)} w\,dA + \frac{d}{dt}\int_{\mathcal{P}} \frac{1}{2}\rho\mathbf{v}\cdot\mathbf{v}\,dV$$

$$\leq \int_{\mathcal{Q}(t)} \left\{ \hat{\mathbf{S}}\cdot\overset{\circ}{\mathbf{F}}_c - \hat{\mathbf{a}}_c\cdot\overset{\circ}{\mathbf{n}} + \nabla_s\cdot\hat{\mathbf{S}}\cdot\mathbf{v}_c \right\} dA + \int_{\partial\mathcal{P}} \mathbf{S}\nu\cdot\mathbf{v}\,dA$$

$$+ \int_{\partial\mathcal{Q}(t)} wV_m\,dL + \int_{\mathcal{Q}(t)} \left[(\nabla_s\cdot\hat{\mathbf{S}})\cdot(\mathbf{F}_c\mathbf{n}) + (\nabla_s\cdot\hat{\mathbf{C}})\cdot\mathbf{n} - 2Hw \right]V_n\,dA, \tag{3.11}$$

where

$$\hat{\mathbf{a}}_c := (\hat{\mathbf{S}}^T\mathbf{F}_c + \hat{\mathbf{C}}^T)\mathbf{n}. \tag{3.12}$$

3.5 Referential localizations and interface driving traction

Application of the surface transport theorem and linear momentum balance to (3.11) yields the

REDUCED DISSIPATION IMBALANCE

$$\frac{d}{dt}\int_{\mathcal{P}} W\,dV \leq \int_{\mathcal{P}} \mathbf{S}\cdot\dot{\mathbf{F}}\,dV + \int_{\mathcal{Q}(t)} \left[(\nabla_s\cdot\hat{\mathbf{S}})\cdot\langle\!\langle\mathbf{F}\mathbf{n}\rangle\!\rangle + (\nabla_s\cdot\hat{\mathbf{C}})\cdot\mathbf{n} \right]V_n\,dA$$

$$- \int_{\mathcal{Q}(t)} \left[\overset{\circ}{w} - \hat{\mathbf{S}}\cdot\overset{\circ}{\mathbf{F}}_c + \hat{\mathbf{a}}_c\cdot\overset{\circ}{\mathbf{n}} \right]. \tag{3.13}$$

Localized away from the interface, this implies that

$$\mathbf{S}\cdot\dot{\mathbf{F}} - \dot{W} \geq 0. \tag{3.14}$$

The local implication at the interface is

$$fV_n - \left[\overset{\circ}{w} - \hat{\mathbf{S}} \cdot \overset{\circ}{\hat{\mathbf{F}}}_c + \hat{\mathbf{a}}_c \cdot \overset{\circ}{\mathbf{n}}\right] \geq 0, \tag{3.15}$$

where

$$f := [\![W]\!] - \langle\!\langle \mathbf{S} \rangle\!\rangle \cdot [\mathbf{F}] + (\nabla_s \cdot \hat{\mathbf{S}}) \cdot \langle\!\langle \mathbf{Fn} \rangle\!\rangle + (\nabla_s \cdot \hat{\mathbf{C}}) \cdot \mathbf{n} \tag{3.16}$$

is the interface *driving traction*. Equation (3.15) was first derived by KNOWLES [15] within a setting devoid of surface fields. GURTIN and STRUTHERS [46] derived (3.15) in its present form, but their work differs from the present development in that, in [46], a more extensive set of postulates leads to a local balance principle with the form of (3.16).

Equations (3.4), (3.10), (3.14) and (3.15) along with the angular momentum localizations,

$$\begin{aligned} \mathbf{S}\mathbf{F}^T &= \mathbf{F}\mathbf{S}^T \\ \hat{\mathbf{S}}\hat{\mathbf{F}}^T &= \hat{\mathbf{F}}\hat{\mathbf{S}}^T, \end{aligned} \tag{3.17}$$

comprise the local field equations for the mechanical theory of dissipative accretion.

4. Hyperelastic materials with interfaces

4.1 Material constitution

The mechanical theory summarized by (3.4), (3.10) and (3.14)–(3.17) is incomplete, since a means of characterizing the bulk and interface of a given material has yet to be provided. This is done by establishing constitutive relationships between the primitive fields and the process kinematics. Though the form of such relations may be quite general, attention for the remainder of this work is restricted to *hyperelastic materials with interfaces*. For such materials, there exist energy response functions $\tilde{W}$ and $\tilde{w}$ such that

$$W = \tilde{W}(\mathbf{F})$$
$$\mathbf{S} = \partial \tilde{W}(\mathbf{F}) \tag{4.1}$$

and

$$w = \tilde{w}(\mathbf{F}_c, \mathbf{n})$$

$$\hat{\mathbf{S}}\mathbf{P} = \partial_1 \tilde{w}(\mathbf{F}_c, \mathbf{n}) \tag{4.2}$$

$$\hat{\mathbf{a}}_c = -\partial_2 \tilde{w}(\mathbf{F}_c, \mathbf{n}),$$

with

$$\tilde{W} : \mathrm{Lin}_+(I\!\!E^3, I\!\!E^3) \overset{c^2}{\to} I\!\!R$$

$$\tilde{w}(\cdot, \mathbf{n}) : \mathrm{Lin}_+(I\!\!E^3, I\!\!E^3) \overset{c^2}{\to} I\!\!R \quad \forall \mathbf{n} \in \mathrm{Unit}(I\!\!E^3), \tag{4.3}$$

and where $\partial_i \phi$ refers to the partial derivative of ϕ with respect to its ith argument. The symbol $\partial \phi$ refers to the derivative of a function ϕ of a single argument. Here and in the following development, $\mathbf{P}$ and $\mathbf{I}$ are treated as elements of $\mathrm{Lin}(I\!\!E^3, \mathbf{n}^\perp)$ and $\mathrm{Lin}(\mathbf{n}^\perp, I\!\!E^3)$, respectively, defined by

$$\mathbf{P}\mathbf{b} = \mathbf{b} - (\mathbf{b} \cdot \mathbf{n})\mathbf{n}, \quad \mathbf{I} = \mathbf{P}^T, \quad \forall \mathbf{b} \in I\!\!E^3. \tag{4.4}$$

The projection and inclusion maps $\bar{\mathbf{P}}, \bar{\mathbf{I}}$ associated with the deformed surface normal $\bar{\mathbf{n}}$ are treated analogously.

For such materials, (3.14) is strictly satisfied, implying that the bulk material does not dissipate energy. The interface is still dissipative, however, with (3.15)

reducing to

$$fV_n \geq 0, \tag{4.5}$$

where the driving traction f is given by (3.16). Accretion is therefore the only way that hyperelastic materials can dissipate energy, as is clear from both (4.5) and the fact that

$$\dot{E} + \dot{K} - P = - \int_{Q(t)} fV_n \, dA \tag{4.6}$$

for such materials. Here E, K, and P are as defined in the mechanical dissipation imbalance.

The interface response functions of (4.1) and (4.2) can be expressed in a more useful form using the following lemma from [46]:

LEMMA 1. Consider a function $\breve{w}$ defined by

$$\breve{w}(\boldsymbol{F}, \mathbf{f}, \mathbf{n}) = \tilde{w}(\boldsymbol{F}\mathbf{P} + \mathbf{f} \otimes \mathbf{n}, \mathbf{n})$$
$$\forall \mathbf{n} \in \mathrm{Unit}(\boldsymbol{E}^3), \quad \forall \mathbf{f} \in \boldsymbol{E}^3, \quad \forall \boldsymbol{F} \in \mathrm{Lin}^{NS}(\mathbf{n}^\perp, \boldsymbol{E}^3). \tag{4.7}$$

Then

$$\partial_1 \breve{w}(\boldsymbol{F}, \mathbf{f}, \mathbf{n}) = \partial_1 \tilde{w}(\boldsymbol{F}\mathbf{P} + \mathbf{f} \otimes \mathbf{n}, \mathbf{n})\mathbf{I}$$
$$\partial_2 \breve{w}(\boldsymbol{F}, \mathbf{f}, \mathbf{n}) = \partial_1 \tilde{w}(\boldsymbol{F}\mathbf{P} + \mathbf{f} \otimes \mathbf{n}, \mathbf{n})\mathbf{n}. \tag{4.8}$$

Lemma 1 and $(4.2)_2$ imply that

$$\hat{\mathbf{S}} = \partial_1 \breve{w}(\boldsymbol{F}, \mathbf{f}, \mathbf{n}) \tag{4.9}$$

and that

$$\partial_2 \breve{w}(\boldsymbol{F}, \mathbf{f}, \mathbf{n}) = \mathbf{0}. \tag{4.10}$$

The surface fields are therefore functions only of $\mathbf{n}$ and $\boldsymbol{F}$, and the surface energy of (4.2) could just as well have depended upon $\mathbf{F}^+$ or $\mathbf{F}^-$; preference has not been given to the bulk on either side of the interface in describing the interfacial fields.

A final step in the material characterization is to express the referential accretive stress $\hat{\mathbf{C}}$ in terms of the surface energy response function $\tilde{w}$. This is facilitated

by introducing $D_{\mathbf{n}}\breve{w}$, the *partial derivative of $\breve{w}$ with respect to $\mathbf{n}$ following the interface*, identified as the unique element of $\mathbf{n}^\perp$ such that

$$D_{\mathbf{n}}\breve{w}(\mathbf{F}, \mathbf{n}) \cdot \mathbf{a} = \left.\frac{d}{d\beta}\breve{w}\left(\mathbf{F}\tilde{\mathbf{Q}}(\mathbf{k}(\beta), \mathbf{n}), \mathbf{k}(\beta)\right)\right|_{\beta=0} \tag{4.11}$$

$$\forall \mathbf{k} : I\!\!R \xrightarrow{c^1} \mathrm{Unit}(I\!\!E^3), \quad \mathbf{k}(0) = \mathbf{n}, \quad \dot{\mathbf{k}}(0) = \mathbf{a},$$

where

$$\tilde{\mathbf{Q}} : \mathrm{Unit}(I\!\!E^3) \times \mathrm{Unit}(I\!\!E^3) \to \mathrm{Orth}_+(I\!\!E^3, I\!\!E^3)$$

is the bilinear map defined by

$$\tilde{\mathbf{Q}}(\mathbf{e}, \mathbf{f})\mathbf{e} = \mathbf{f}, \quad \tilde{\mathbf{Q}}(\mathbf{e}, \mathbf{f})\mathbf{g} = \mathbf{g} \qquad \forall \{\mathbf{e}, \mathbf{f}\} \in \mathrm{Unit}(I\!\!E^3) \times \mathrm{Unit}(I\!\!E^3),$$

with $\mathbf{g} \cdot \mathbf{e} = \mathbf{g} \cdot \mathbf{f} = 0$. Then, as shown in [46],

$$D_{\mathbf{n}}\breve{w}(I\!\!F, \mathbf{f}, \mathbf{n}) = \partial_2 \breve{w}(I\!\!F\mathbf{P} + \mathbf{f} \otimes \mathbf{n}, \mathbf{n}) + [\partial_1 \breve{w}(I\!\!F, \mathbf{f}, \mathbf{n})]^T \mathbf{f} - I\!\!F^T \partial_2 \breve{w}(I\!\!F, \mathbf{f}, \mathbf{n}). \tag{4.12}$$

Since

$$\hat{\mathbf{C}} = I\!\!P\hat{\mathbf{C}} + \mathbf{n} \otimes \hat{\mathbf{C}}^T \mathbf{n}, \tag{4.13}$$

(3.10) and (3.12) and the fact that $\mathbf{PI} = \mathbf{1}_s$ combine to give

$$\hat{\mathbf{C}} = w\mathbf{I} - I\!\!F^T \hat{\mathbf{S}} + \mathbf{n} \otimes \left(\hat{\mathbf{a}}_c - \hat{\mathbf{S}}^T \mathbf{F}_c \mathbf{n}\right). \tag{4.14}$$

Equations (4.2), (4.7), (4.9) and (4.12) then yield

$$\hat{\mathbf{C}} = \breve{w}(I\!\!F, \mathbf{f}, \mathbf{n})\mathbf{I} - I\!\!F^T \partial_1 \breve{w}(I\!\!F, \mathbf{f}, \mathbf{n}) - \mathbf{n} \otimes D_{\mathbf{n}}\breve{w}(I\!\!F, \mathbf{f}, \mathbf{n}). \tag{4.15}$$

Equations (4.9), (4.10) and (4.15) admit the following characterization of hyperelastic materials with interfaces:

$$\begin{aligned} W &= \tilde{W}(\mathbf{F}) \\ \mathbf{S} &= \partial \tilde{W}(\mathbf{F}), \end{aligned} \tag{4.16}$$

and

$$w = \breve{w}(I\!\!F, \mathbf{n})$$

$$\hat{\mathbf{S}} = \partial_1 \breve{w}(I\!\!F, \mathbf{n}) \tag{4.17}$$

$$\hat{\mathbf{C}} = \breve{w}(I\!\!F, \mathbf{n})\mathbf{I} - I\!\!F^T \partial_1 \breve{w}(I\!\!F, \mathbf{n}) - \mathbf{n} \otimes D_{\mathbf{n}}\breve{w}(I\!\!F, \mathbf{n}).$$

Note that the response of the system is independent of the scalar c introduced in (3.3). The *tangential component* of $\hat{\mathbf{C}}$ refers to $\mathbf{P}\hat{\mathbf{C}}$, and only the first two terms in the above expression for $\hat{\mathbf{C}}$ are represented in its tangential component since $\mathbf{Pn} = 0$. The last term in $(4.17)_3$ is referred to as the *normal component* of the accretive stress and is equivalent to $\mathbf{n} \otimes \hat{\mathbf{C}}^T \mathbf{n}$.

4.2 A kinetic relation for interfaces

The mechanical theory of hyperelastic materials summarized by (3.4), (3.17), (4.5) and (4.16)–(4.17) is still incomplete. As shown by ERICKSEN [12] and ABEYARATNE and KNOWLES [21–23, 26] for the case of no surface fields, there are settings for which the location of the interface cannot be determined uniquely for prescribed boundary data. Abeyaratne and Knowles suggest that this may be interpreted as a constitutive deficiency. Motivated by the internal variable work of RICE [43, 44] and the form of (4.5), they offer a simple remedy in the form of a constitutive relation between the driving *traction* f and the accretive velocity of the interface V_n:

$$
\begin{aligned}
&V_n = \hat{V}(f), \\
&\hat{V} : I\!\!R \to I\!\!R, \quad \hat{V}(f)f \geq 0 \quad \forall f \in I\!\!R.
\end{aligned}
\tag{4.18}
$$

Equation $(4.18)_1$ is referred to as a *kinetic relation* with the inequality restricting $\hat{V}$ imposed by the dissipation imbalance (4.5). Supplementing the system postulates and material constitution with such a relation has been shown, in certain settings, to resolve the uniqueness problem [23, 26, 28–30]. Though developed without considering surface fields, the rationale for adopting a kinetic relation is still valid within settings that include interfacial structure. Such a constitutive remedy is therefore adopted in the present work. It should be noted, however, that GURTIN and STRUTHERS [46] have *derived* an equation with the form of $(4.18)_1$ from a more elaborate set of balance postulates.

4.3 Mechanical equivalence

Consider two lattice elements $\mathcal{K}_1$ and $\mathcal{K}_2$ with respect to which a body is hyperelastic, that are related by linear transformation $\mathbf{H}$, where $\mathcal{K}_2 = \mathbf{H} \circ \mathcal{K}_1$. These two reference configurations are said to be *mechanically equivalent* if first,

$$\rho_1(\mathbf{x},t) = \rho_2(\mathbf{Hx},t) \quad \forall \mathbf{x} \in \mathcal{R}_1(t) \backslash \mathcal{S}_1(t), \quad \forall t \in \mathcal{T} \tag{4.19}$$

and, second, they are characterized by the same response functions:

$$\tilde{W}_2 = \tilde{W}_1, \qquad \check{w}_2 = \check{w}_1. \tag{4.20}$$

By virtue of the construction of referential fields given in section 3.3, the following formulae relate mass density and energy fields independent of any constitutive considerations:

$$\begin{aligned} \rho_2(\mathbf{x},t) &= \mathrm{Det}(\mathbf{H})\rho_1(\mathbf{Hx},t) \\ W_2(\mathbf{x},t) &= \frac{1}{\mathrm{Det}(\mathbf{H})}W_1(\mathbf{Hx},t) \end{aligned} \quad \forall \mathbf{x} \in \mathcal{R}_1 \backslash \mathcal{S}_1(t), \quad \forall t \in \mathcal{T} \tag{4.21}$$

and

$$w_2(\mathbf{x},t) = \frac{\|\mathbf{H}^T\mathbf{n}(\mathbf{x},t)\|}{\mathrm{Det}(\mathbf{H})}w_1(\mathbf{Hx},t) \quad \forall \mathbf{x} \in \mathcal{S}_1(t), \quad \forall t \in \mathcal{T}. \tag{4.22}$$

Equations (4.19)-(4.22) collectively imply that two reference configurations are mechanically equivalent if and only if

$$\begin{aligned} &\mathrm{Det}(\mathbf{H}) = 1 \\ &\tilde{W}_1(\mathbf{F}) = \tilde{W}_1(\mathbf{HF}) \\ &\tilde{w}_1(\mathbf{F},\mathbf{n}) = \|\mathbf{H}^T\mathbf{n}\|\check{w}_1\left(\mathbf{FH},\frac{\mathbf{H}^T\mathbf{n}}{\|\mathbf{H}^T\mathbf{n}\|}\right) \end{aligned} \quad \forall \mathbf{F} \in \mathrm{Lin}_+(I\!\!E^3,I\!\!E^3), \quad \forall \mathbf{n} \in \mathrm{Unit}(I\!\!E^3).$$

$$\tag{4.23}$$

Define the *material symmetry group* $\mathcal{G}_\kappa$ of a latticed body with respect to lattice element $\mathcal{K}$ to be the set of all lattice elements that are mechanically equivalent to $\mathcal{K}$. If $\mathcal{G}_\kappa = \mathrm{Unim}(I\!\!E^3,I\!\!E^3)$, the material is called a *fluid*. If $\mathcal{G}_\kappa = \mathrm{Orth}_+(I\!\!E^3,I\!\!E^3)$, the material is called a *solid*.

The kinetic relation does not play a role in determining the mechanical equivalence of two lattice elements. An appropriate change of configuration formula can, however, be established. Let J_H and j_H be the bulk and surface determinants associated with the linear transformation $\mathbf{H}$. Then

$$V_n^{(2)} = \frac{J_H}{j_H} V_n^{(1)} \tag{4.24}$$

and

$$f_1 = J_H f_2 \tag{4.25}$$

so that

$$\hat{V}_2\left(\frac{f}{J_H}\right) = \frac{J_H}{j_H} \hat{V}_1(f) \qquad \forall f \in I\!R. \tag{4.26}$$

4.4 The role of accretive stress

Recall that the local power expenditure associated with $\hat{\mathbf{C}}$ is given by $\hat{\mathbf{C}}\mathbf{m} \cdot \mathbf{V}$. For hyperelastic materials, then, $(4.17)_3$ implies that

$$\hat{\mathbf{C}}\mathbf{m} \cdot \mathbf{V} = \left\{ \breve{w} - \left[(\hat{\mathbf{F}}^T \partial_1 \breve{w})\mathbf{m} \right] \cdot \mathbf{m} \right\} V_m -- \left[(D_n \breve{w}) \cdot \mathbf{m} \right] V_n. \tag{4.27}$$

The first term represents power expended in extending the interface boundary via tangential accretion. The second term represents a power expenditure accompanying changes in interfacial orientation in association with normal accretion. The accretive traction has a physically meaningful relation to the symmetry exhibited by the interface and is embodied in the following

THEOREM ON FLUID-SURFACES.

(A) For fluids:

    (i) $\breve{w} = \bar{\sigma}$, a constant;

    (ii) $\hat{\mathbf{C}} = \mathbf{0}$; and

    (iii) $\hat{\mathbf{T}} = \bar{\sigma}\mathbf{1}_s$.

(B) For a hyperelastic bodies that do not support an accretive stress:

(i) $\bar{w} = \bar{\sigma}$, a constant; and

(ii) $\hat{T} = \bar{\sigma}1_s$.

(C) For a hyperelastic material with constant interfacial energy per unit area:

(i) $\hat{T} = \bar{\sigma}1_s$; and

(ii) $\hat{C} = 0$.

(A) is due to GURTIN and STRUTHERS [46], while (B) and (C) are new.

Proof.(B) For $\hat{C} = 0$, the tension-energy theorem of section 3.4 implies that

$$I\!F^T\hat{S} = w1_s. \tag{4.28}$$

In terms of $\hat{T}$, this is equivalent to

$$w1_s = jI\!F^T\bar{I}\hat{T}\hat{F}^{-T} = j\hat{F}^T\hat{T}\hat{F}^{-T}.$$

Therefore,

$$\hat{T} = \frac{w}{j}\hat{F}^{-T}1_s\hat{F}^T = \bar{w}1_s.$$

Equation (ii) is therefore proved once (i) is established. It may be shown that (4.28) is equivalent to

$$\hat{S} = w\bar{I}\hat{F}^{-T}. \tag{4.29}$$

But for hyperelastic materials, $(4.17)_2$ gives

$$\hat{S} = \partial_1\check{w}(I\!F, n). \tag{4.30}$$

Now let

$$\bar{\sigma}(I\!F, n) := \frac{1}{j}\check{w}(I\!F, n)$$

so that

$$\partial_1\check{w}(I\!F, n) = j\bar{I}\hat{F}^{-T}\bar{\sigma}(I\!F, n) + j\partial_1\bar{\sigma}(I\!F, n). \tag{4.31}$$

Here use has been made of the identity,

$$\partial_1 \breve{\jmath}(I\!\!F, \mathbf{n}) = j \dot{\mathbf{I}} \hat{\mathbf{F}}^{-T} \tag{4.32}$$

from [46], with $\breve{\jmath}(I\!\!F, \mathbf{n}) = j$. Equations (4.29)-(4.31) then imply that

$$\breve{w}(I\!\!F, \mathbf{n}) \dot{\mathbf{I}} \hat{\mathbf{F}}^{-T} = j \bar{\sigma}(I\!\!F, \mathbf{n}) \dot{\mathbf{I}} \hat{\mathbf{F}}^{-T} + j \partial_1 \bar{\sigma}(I\!\!F, \mathbf{n}).$$

Therefore,

$$\partial_1 \bar{\sigma}(I\!\!F, \mathbf{n}) = \mathbf{0}. \tag{4.33}$$

$\hat{\mathbf{C}} = \mathbf{0}$ also implies that $\hat{\mathbf{C}}^T \mathbf{n} = \mathbf{0}$ which, by $(4.17)_3$, gives that

$$0 = D_{\mathbf{n}} \breve{w}(I\!\!F, \mathbf{n}) = \left[D_{\mathbf{n}} \breve{\jmath}(\mathbf{F}, \mathbf{n}) \right] \bar{\sigma}(I\!\!F, \mathbf{n}) + \breve{\jmath}(\mathbf{F}, \mathbf{n}) \left[D_{\mathbf{n}} \bar{\sigma}(I\!\!F, \mathbf{n}) \right], \tag{4.34}$$

where

$$\breve{\jmath}(\mathbf{F}, \mathbf{n}) := \frac{\mathrm{Det}(\mathbf{F})}{\| \mathbf{F}^{-T} \mathbf{n} \|}$$

from $(2.19)_2$. But following the definition of $D_{\mathbf{n}}(\cdot)$ given by (4.11),

$$\begin{aligned}
D_{\mathbf{n}} \breve{\jmath}(\mathbf{F}, \mathbf{n}) &= \frac{d}{d\beta} \left\{ \frac{\mathrm{Det}\left[\mathbf{F} \tilde{\mathbf{Q}}(\mathbf{k}(\beta), \mathbf{n}) \right]}{\| \left[\mathbf{F} \tilde{\mathbf{Q}}(\mathbf{k}(\beta), \mathbf{n}) \right]^{-T} \mathbf{k}(\beta) \|} \right\} \Bigg|_{\beta=0} \\
&= \frac{d}{d\beta} \left\{ \frac{\mathrm{Det}(\mathbf{F})}{\| \mathbf{F}^{-T} \tilde{\mathbf{Q}}(\mathbf{k}(\beta), \mathbf{n}) \mathbf{k}(\beta) \|} \right\} \Bigg|_{\beta=0} \\
&= \frac{d}{d\beta} \left\{ \frac{\mathrm{Det}(\mathbf{F})}{\| \mathbf{F}^{-T} \mathbf{n} \|} \right\} \Bigg|_{\beta=0} \\
&= 0.
\end{aligned} \tag{4.35}$$

Since

$$D_{\mathbf{n}} \breve{\jmath}(I\!\!F, \mathbf{n}) = D_{\mathbf{n}} \breve{\jmath}(I\!\!F \mathbf{P} + \mathbf{f} \otimes \mathbf{n}, \mathbf{n})$$

by construction, (4.34) and (4.35) imply that

$$D_{\mathbf{n}} \bar{\sigma}(I\!\!F, \mathbf{n}) = \mathbf{0}.$$

Use of (4.7), (4.8), and (4.12) with $\bar{\sigma}$ in place of w then gives that $\bar{\sigma}$ must be a constant-valued function. Thus, $\breve{w} = \bar{\sigma}$, a constant. $\qquad \square$

Proof.(C) $\bar{w} = \bar{\sigma}$ is equivalent to $w = j\bar{\sigma}$ so that $\hat{\mathbf{S}} = j\bar{\sigma}\mathbf{I}\hat{\mathbf{F}}^{-T}$. Expression of this result in terms of $\hat{\mathbf{T}}$ yields $\hat{\mathbf{T}} = \bar{\sigma}\mathbf{1}_s$ and also implies that

$$\mathbf{I}\mathbf{F}^T\hat{\mathbf{S}} = j\bar{\sigma}\mathbf{I} = w\mathbf{I}.$$

From (4.30) and the fact that $w = j\bar{\sigma}$,

$$D_{\mathbf{n}}\breve{w}(\mathbf{F}, \mathbf{n}) = \mathbf{0}.$$

Substitution of this result and (4.33) into (4.17)$_3$ yields

$$\hat{\mathbf{C}} = w\mathbf{I} - w\mathbf{I} - \mathbf{n} \otimes \mathbf{0} = \mathbf{0}. \qquad \square$$

Part (A) indicates that fluids cannot support an accretive stress, though the converse of this does not hold in general. Parts (B) and (C), on the other hand, do not depend upon the mechanical symmetry of the body. They imply that, independent of the constitution of the bulk, an interface exhibits a *fluid nature*—that is, surface energy and surface tension characterized by the same scalar constant—if and only if $\hat{\mathbf{C}} = \mathbf{0}$. Thus, the accretive stress accounts for special properties of interfaces exibiting a solid nature that are not associated with their fluid-like counterparts.

5. Isotropic, hyperelastic materials with interfaces

A standard result in continuum mechanics asserts that hyperelastic materials are isotropic with respect to a given reference configuration if and only if the bulk energy can be represented by a function of the three fundamental scalar invariants of the right Cauchy-Green tensor $C := F^T F$ or its square root U. These scalar invariants are defined as

$$
\begin{aligned}
I_1(U) &:= \text{Trace}(U) \\
I_2(U) &:= \frac{1}{2}\big[(\text{Trace}(U))^2 - \text{Trace}(U^2)\big] \qquad \forall U \in \text{Sym}^+(I\!\!E^3), \\
I_3(U) &:= \text{Det}(U)
\end{aligned}
\tag{5.1}
$$

so that, in the absence of surface fields, a hyperelastic material is isotropic if and only if it is characterized by

$$
\begin{aligned}
W &= \breve{W}(I_1, I_2, I_3) \\
S &= (\partial_1\breve{W} + I_1\partial_2\breve{W})FU^{-1} - (\partial_2\breve{W})F + (I_3\partial_3\breve{W})F^{-\tau} \\
T &= \frac{1}{I_3}(\partial_1\breve{W} + I_1\partial_2\breve{W})V - \frac{1}{I_3}(\partial_2\breve{W})V^2 + (\partial_3\breve{W})1,
\end{aligned}
\tag{5.2}
$$

where

$$
I_k := I_k(U) = I_k(V), \quad U := \sqrt{F^T F}, \quad \text{and} \quad V := \sqrt{F F^T}.
\tag{5.3}
$$

Material isotropy also imposes restrictions on the interfacial response functions, and the elucidation of these restrictions is central to this work. One such restriction is on the accretive surface stress $\hat{C}$ and is a direct result of the following

PROPOSITION 1. Material isotropy implies that $D_n\breve{w} = 0$.

Proof. By (4.23), isotropy implies that

$$
\breve{w}(F, n) = \breve{w}(FQ, Q^\tau n)
$$

$$
\forall Q \in \text{Orth}_+(I\!\!E^3, I\!\!E^3), \quad \forall F \in \text{Lin}_+(I\!\!E^3, I\!\!E^3), \quad \forall n \in \text{Unit}(I\!\!E^3).
\tag{5.4}
$$

Recalling (4.11), let

$$
Q = \tilde{Q}(k(\beta), n)
$$

for some

$$\mathbf{k} : I\!\!R \overset{c^1}{\hookrightarrow} \text{Unit}(I\!\!E^3), \quad \mathbf{k}(0) = \mathbf{n}.$$

Then,

$$\tilde{\mathbf{Q}}^T(\mathbf{k}(\beta), \mathbf{n})\mathbf{n} = \mathbf{k}(\beta) \tag{5.5}$$

so that (5.4) implies that

$$\tilde{w}\bigg(\mathbf{F}\tilde{\mathbf{Q}}(\mathbf{k}(\beta), \mathbf{n}), \mathbf{k}(\beta)\bigg) = \tilde{w}(\mathbf{F}, \mathbf{n}) \quad \forall \beta. \tag{5.6}$$

Therefore,

$$\frac{d}{d\beta}\tilde{w}\bigg(\mathbf{F}\tilde{\mathbf{Q}}(\mathbf{k}(\beta), \mathbf{n}), \mathbf{k}(\beta)\bigg) = \frac{d}{d\beta}\tilde{w}(\mathbf{F}, \mathbf{n}) = 0.$$

Thus, by the definition of $D_{\mathbf{n}}\tilde{w}$ given by (4.11), $D_{\mathbf{n}}\tilde{w} = D_{\mathbf{n}}\breve{w} = 0$. $\qquad \square$

Prop. 1 implies that the accretive stress of isotropic, hyperelastic materials does not have a normal component. This is clear from (4.17). In light of this result and using (4.27), it may be concluded that any work performed by $\hat{\mathbf{C}}$ to reorient the interface must be due to material anisotropy since the last term in (4.27) vanishes for isotropic bodies. LEO and SEKERKA [48] conclude that such a work term should be present for anisotropic, hyperelastic materials, and the idea is also in line with the earlier work of CAHN and HOFFMAN [49] and HOFFMAN and CAHN [50], who adopted a capillary traction vector to account for anisotropic effects in non-deformable media. In fact, consideration of such a work term can be traced back to HERRING [41, 42].

Attention is next turned to the representation of interfacial fields in terms of the scalar invariants of the surface deformation gradient. An *isotropic, scalar function ϕ* is characterized by the property that

$$\phi(\hat{\mathbf{Q}}^T \hat{\mathbf{U}} \hat{\mathbf{Q}}, \mathbf{n}) = \phi(\hat{\mathbf{U}}, \mathbf{n})$$

$$\forall \hat{\mathbf{U}} \in \text{Sym}^+(\mathbf{n}^\perp), \quad \forall \hat{\mathbf{Q}} \in \text{Orth}_+(\mathbf{n}^\perp, \mathbf{n}^\perp), \quad \forall \mathbf{n} \in \text{Unit}(I\!\!E^3). \tag{5.7}$$

Such functions admit an equivalent representation in terms of the two fundamental scalar invariants of their first argument—a property expressed in the following

PROPOSITION 2. If ϕ is an isotropic, scalar function, then there exists a function, $\hat{\phi} : \hat{\mathcal{I}} \times \text{Unit}(\mathbb{E}^3) \to \mathbb{R}$ such that

$$\phi(\hat{\mathbf{U}}, \mathbf{n}) = \hat{\phi}(i(\hat{\mathbf{U}}), j(\hat{\mathbf{U}}), \mathbf{n})$$
$$\forall \hat{\mathbf{U}} \in \text{Sym}^+(\mathbf{n}^\perp), \quad \forall \mathbf{n} \in \text{Unit}(\mathbb{E}^3), \tag{5.8}$$

where

$$\hat{\mathcal{I}} := \left\{ (\zeta_1, \zeta_2) \,\middle|\, (\zeta_1, \zeta_2) \in \mathbb{R}^2_+, \quad (4\zeta_2 - \zeta_1^2) < 0 \right\} \tag{5.9}$$

and

$$i(\hat{\mathbf{U}}) := \text{Trace}(\hat{\mathbf{U}}), \qquad j(\hat{\mathbf{U}}) := \text{Det}(\hat{\mathbf{U}}). \tag{5.10}$$

This proposition is proved with the help of the following two lemmas.

LEMMA 2. $(\zeta_1, \zeta_2) \in \mathbb{R}^2_+$ coincide, respectively, with $i(\hat{\mathbf{A}})$ and $j(\hat{\mathbf{A}})$ for some $\hat{\mathbf{A}} \in \text{Sym}^+(\mathbf{n}^\perp)$ if and only if $(\zeta_1, \zeta_2) \in \hat{\mathcal{I}}$, with $\hat{\mathcal{I}}$ as defined in (5.9).

Proof. Suppose $\hat{\mathbf{A}} \in \text{Sym}^+(\mathbf{n}^\perp)$. Then $\hat{\mathbf{A}}$ has two, real, positive eigenvalues $\hat{\lambda}$ satisfying the characteristic equation

$$p(\hat{\lambda}) = -\hat{\lambda}^2 + i(\hat{\mathbf{A}})\hat{\lambda} - j(\hat{\mathbf{A}}) = 0.$$

Application of the quadratic formula then reveals that $\big(i(\hat{\mathbf{A}}), j(\hat{\mathbf{A}})\big) \in \hat{\mathcal{I}}$. Conversely, suppose $(\zeta_1, \zeta_2) \in \hat{\mathcal{I}}$. Then

$$-\hat{\lambda}^2 + \zeta_1 \hat{\lambda} - \zeta_2 = 0$$

has two positive roots λ_1, λ_2 and $\zeta_1 = \lambda_1 + \lambda_2$ and $\zeta_2 = \lambda_1 \lambda_2$. Construct $\hat{\mathbf{A}} \in \text{Sym}^+(\mathbf{n}^\perp)$ such that it has a component representation in its principal, rectilinear, Cartesian coordinate basis of

$$[\hat{\mathbf{A}}] = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}.$$

Clearly, $i(\hat{\mathbf{A}}) = \zeta_1$ and $j(\hat{\mathbf{A}}) = \zeta_2$. $\qquad\qquad \square$

LEMMA 3. Let $\hat{\mathbf{A}}, \hat{\mathbf{B}} \in \text{Sym}^+(\mathbf{n}^\perp)$. Then $i(\hat{\mathbf{A}}) = i(\hat{\mathbf{B}})$, $j(\hat{\mathbf{A}}) = j(\hat{\mathbf{B}})$ if and only if there exists a $\hat{\mathbf{Q}} \in \text{Orth}_+(\mathbf{n}^\perp, \mathbf{n}^\perp)$, such that $\hat{\mathbf{B}} = \hat{\mathbf{Q}}^T \hat{\mathbf{A}} \hat{\mathbf{Q}}$.

Proof. Suppose $\hat{\mathbf{B}} = \hat{\mathbf{Q}}^T \hat{\mathbf{A}} \hat{\mathbf{Q}}$, $\hat{\mathbf{Q}} \in \text{Orth}_+(\mathbf{n}^\perp, \mathbf{n}^\perp)$. Then

$$i(\hat{\mathbf{B}}) = \langle \hat{\mathbf{B}}, \mathbf{1}_s \rangle = \langle \hat{\mathbf{Q}}^T \hat{\mathbf{A}} \hat{\mathbf{Q}}, \mathbf{1}_s \rangle$$
$$= \langle \hat{\mathbf{A}}, \hat{\mathbf{Q}} \hat{\mathbf{Q}}^T \rangle = \langle \hat{\mathbf{A}}, \mathbf{1}_s \rangle = i(\hat{\mathbf{A}}).$$

Also,

$$j(\hat{\mathbf{B}}) = j(\hat{\mathbf{Q}}^T \hat{\mathbf{A}} \hat{\mathbf{Q}}) = j(\hat{\mathbf{Q}}^T) j(\hat{\mathbf{A}}) j(\hat{\mathbf{Q}}) = j(\hat{\mathbf{A}}).$$

Conversely, suppose $i(\hat{\mathbf{A}}) = i(\hat{\mathbf{B}})$ and $j(\hat{\mathbf{A}}) = j(\hat{\mathbf{B}})$. Then the eigenvalues of $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ coincide since they are both given by the characteristic polynomial

$$-\hat{\lambda}^2 + i\hat{\lambda} - j = 0.$$

Let $\{\mathbf{e}_1, \mathbf{e}_2\}$ and $\{\mathbf{e}_1', \mathbf{e}_2'\}$ be the associated principal bases for $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$, respectively. Then there exists a $\hat{\mathbf{Q}} \in \text{Orth}_+(\mathbf{n}^\perp, \mathbf{n}^\perp)$, such that $\hat{\mathbf{Q}} \mathbf{e}_\alpha' = \mathbf{e}_\alpha$, $\alpha = 1, 2$. Thus ,

$$\hat{\mathbf{B}} \mathbf{e}_\alpha' = \lambda_\alpha \mathbf{e}_\alpha' = \lambda_\alpha \hat{\mathbf{Q}}^T \mathbf{e}_\alpha = \hat{\mathbf{Q}}^T \hat{\mathbf{A}} \mathbf{e}_\alpha = \hat{\mathbf{Q}}^T \hat{\mathbf{A}} \hat{\mathbf{Q}} \mathbf{e}_\alpha', \quad \alpha = 1, 2,$$

implying that $\hat{\mathbf{B}} = \hat{\mathbf{Q}}^T \hat{\mathbf{A}} \hat{\mathbf{Q}}$. $\qquad\qquad\qquad \Box$

Suppose there exists a function $\tilde{\phi} : \hat{\mathcal{I}} \times \text{Unit}(I\!E^3) \to I\!R$ such that

$$\phi(\hat{\mathbf{U}}, \mathbf{n}) = \tilde{\phi}(i(\hat{\mathbf{U}}), j(\hat{\mathbf{U}}), \mathbf{n}) \quad \forall \hat{\mathbf{U}} \in \text{Sym}^+(\mathbf{n}^\perp), \quad \forall \mathbf{n} \in \text{Unit}(I\!E^3).$$

Then by Lemma 3,

$$\phi(\hat{\mathbf{U}}, \mathbf{n}) = \tilde{\phi}(i(\hat{\mathbf{Q}}^T \hat{\mathbf{U}} \hat{\mathbf{Q}}), j(\hat{\mathbf{Q}}^T \hat{\mathbf{U}} \hat{\mathbf{Q}}), \mathbf{n})$$
$$= \phi(\hat{\mathbf{Q}}^T \hat{\mathbf{U}} \hat{\mathbf{Q}}, \mathbf{n}) \quad \forall \hat{\mathbf{Q}} \in \text{Orth}_+(\mathbf{n}^\perp, \mathbf{n}^\perp).$$

Therefore, ϕ is an isotropic, scalar function. Conversely, if ϕ is an isotropic, scalar function then by Lemmas 2 and 3 there exists a single-valued function, $\tilde{\phi} : \hat{\mathcal{I}} \times \text{Unit}(I\!E^3) \to I\!R$, such that

$$\phi(\hat{\mathbf{U}}, \mathbf{n}) = \tilde{\phi}(i(\hat{\mathbf{U}}), j(\hat{\mathbf{U}}), \mathbf{n}) \quad \forall \hat{\mathbf{U}} \in \text{Sym}^+(\mathbf{n}^\perp), \quad \forall \mathbf{n} \in \text{Unit}(I\!E^3).$$

Prop. 2 is therefore established. It is will now be used to show that the interfaces of isotropic, hyperelastic materials may be characterized by two scalar invariants of the interface deformation as given by the

INTERFACE REPRESENTATION THEOREM.

Hyperelastic materials whose bulk is characterized by (5.2) are isotropic if and only if the interfacial energy can be represented by a function $\hat{w} : \hat{\mathcal{I}} \to I\!\!R$, such that

$$\breve{w}(I\!\!F, \mathbf{n}) = \hat{w}\big(i(\hat{\mathbf{U}}), j(\hat{\mathbf{U}})\big)$$
$$\forall I\!\!F \in \mathrm{Lin}^{NS}(\mathbf{n}^{\perp}, I\!\!E^3), \quad \forall \mathbf{n} \in \mathrm{Unit}(I\!\!E^3), \tag{5.11}$$

where

$$\hat{\mathbf{U}} := \sqrt{I\!\!F^T I\!\!F} = \sqrt{\hat{\mathbf{F}}^T \hat{\mathbf{F}}}. \tag{5.12}$$

Proof. That the representation given by (5.11) is possible for all isotropic materials is proved with the help of two lemmas. The first establishes that the interfacial energy of isotropic, hyperelastic materials may be characterized by an isotropic, scalar function while the second lemma allows the orientation dependence of the surface energy response function to be dropped.

LEMMA 4. For isotropic, hyperelastic materials the referential, interfacial energy can be represented by an isotropic, scalar function

$$\breve{w}(\cdot, \mathbf{n}) : \mathrm{Sym}^+(\mathbf{n}^{\perp}) \to I\!\!R, \quad \forall \mathbf{n} \in \mathrm{Unit}(I\!\!E^3).$$

Proof. Galilean objectivity implies that

$$\breve{w}(\mathbf{Q}\mathbf{F}\mathbf{I}, \mathbf{n}) = \breve{w}(\mathbf{F}\mathbf{I}, \mathbf{n}) \quad \forall \mathbf{Q} \in \mathrm{Orth}_+(I\!\!E^3, I\!\!E^3), \quad \forall \mathbf{F} \in \mathrm{Lin}_+(I\!\!E^3, I\!\!E^3),$$
$$\forall \mathbf{n} \in \mathrm{Unit}(I\!\!E^3), \tag{5.13}$$

with $\mathbf{I}$ the inclusion map associated with $\mathbf{n}^{\perp}$.

By the polar decomposition theorem, there exist unique

$$\hat{\mathbf{U}} \in \mathrm{Sym}^+(\mathbf{n}^{\perp}), \quad \hat{\mathbf{Q}} \in \mathrm{Orth}_+(\mathbf{n}^{\perp}, \mathbf{n}^{\perp}),$$

such that $\hat{\mathbf{F}} = \hat{\mathbf{Q}}\hat{\mathbf{U}}$ for every $\hat{\mathbf{F}} \in \mathrm{Lin}_+(\mathbf{n}^\perp, \bar{\mathbf{n}}^\perp)$.

Consider a particular linear transformation

$$\mathbf{Q} = \mathbf{I}\hat{\mathbf{Q}}^T\bar{\mathbf{P}} + \mathbf{n} \otimes \bar{\mathbf{n}}.$$

Note that this $\mathbf{Q}$ is in $\mathrm{Orth}_+(\mathbb{E}^3, \mathbb{E}^3)$ since

$$\mathbf{Q}\mathbf{Q}^T = (\mathbf{I}\hat{\mathbf{Q}}^T\bar{\mathbf{P}} + \mathbf{n} \otimes \bar{\mathbf{n}})(\bar{\mathbf{I}}\hat{\mathbf{Q}}\mathbf{P} + \bar{\mathbf{n}} \otimes \mathbf{n})$$

$$= \mathbf{I}\hat{\mathbf{Q}}^T\bar{\mathbf{P}}\bar{\mathbf{I}}\hat{\mathbf{Q}}\mathbf{P} + \mathbf{I}\hat{\mathbf{Q}}^T\bar{\mathbf{P}}\bar{\mathbf{n}} \otimes \mathbf{n} + (\mathbf{n} \otimes \bar{\mathbf{n}})\bar{\mathbf{I}}\hat{\mathbf{Q}}\mathbf{P} + (\mathbf{n} \otimes \bar{\mathbf{n}})(\bar{\mathbf{n}} \otimes \mathbf{n})$$

$$= \mathbf{I}\hat{\mathbf{Q}}^T\mathbf{1}_{\bar{s}}\hat{\mathbf{Q}}\mathbf{P} + \mathbf{n} \otimes \mathbf{n}$$

$$= \mathbf{I}\hat{\mathbf{Q}}^T\hat{\mathbf{Q}}\mathbf{P} + \mathbf{n} \otimes \mathbf{n} = \mathbf{I}\mathbf{P} + \mathbf{n} \otimes \mathbf{n} = \mathbf{1}.$$

For this choice of $\mathbf{Q}$,

$$\mathbf{Q}\mathbf{F}\mathbf{I} = \mathbf{Q}\bar{\mathbf{I}}\hat{\mathbf{F}} = \mathbf{Q}\bar{\mathbf{I}}\hat{\mathbf{Q}}\hat{\mathbf{U}} = (\mathbf{I}\hat{\mathbf{Q}}^T\bar{\mathbf{P}} + \mathbf{n} \otimes \bar{\mathbf{n}})\bar{\mathbf{I}}\hat{\mathbf{Q}}\hat{\mathbf{U}}$$

$$= \mathbf{I}\hat{\mathbf{Q}}^T\bar{\mathbf{P}}\bar{\mathbf{I}}\hat{\mathbf{Q}}\hat{\mathbf{U}} + (\mathbf{n} \otimes \bar{\mathbf{n}})\bar{\mathbf{I}}\hat{\mathbf{Q}}\hat{\mathbf{U}} = \mathbf{I}\hat{\mathbf{Q}}^T\mathbf{1}_{\bar{s}}\hat{\mathbf{Q}}\hat{\mathbf{U}} = \mathbf{I}\hat{\mathbf{U}}.$$

Thus, Galilean objectivity implies that

$$\breve{w}(\mathbf{F}\mathbf{I}, \mathbf{n}) = \breve{w}(\mathbf{I}\hat{\mathbf{U}}, \mathbf{n}) \quad \forall \mathbf{F} \in \mathrm{Lin}_+(\mathbb{E}^3, \mathbb{E}^3), \quad \forall \mathbf{n} \in \mathrm{Unit}(\mathbb{E}^3), \qquad (5.14)$$

with

$$\hat{\mathbf{U}} = \sqrt{\mathbb{F}^T\mathbb{F}} = \sqrt{\hat{\mathbf{F}}^T\hat{\mathbf{F}}},$$

and where $\mathbb{F}$ and $\hat{\mathbf{F}}$ are as defined as in section 2.5.

Now suppose that $\mathbf{Q} := \mathbf{I}\hat{\mathbf{Q}}\mathbf{P} + \mathbf{n} \otimes \mathbf{n}$ with $\hat{\mathbf{Q}} \in \mathrm{Orth}_+(\mathbf{n}^\perp, \mathbf{n}^\perp)$. Then $\mathbf{Q}^T\mathbf{Q} = \mathbf{1}$ and $\hat{\mathbf{Q}} = \mathbf{P}\mathbf{Q}\mathbf{I}$. From (5.13) and (5.14),

$$\breve{w}(\mathbf{F}\mathbf{I}, \mathbf{n}) = \breve{w}(\mathbf{I}\hat{\mathbf{U}}, \mathbf{n}) = \breve{w}(\mathbf{Q}\mathbf{I}\hat{\mathbf{U}}, \mathbf{n}). \qquad (5.15)$$

But for the $\mathbf{Q}$ chosen,

$$\mathbf{Q}\mathbf{I}\hat{\mathbf{U}} = (\mathbf{I}\hat{\mathbf{Q}}\mathbf{P} + \mathbf{n} \otimes \mathbf{n})\mathbf{I}\hat{\mathbf{U}} = \mathbf{I}\hat{\mathbf{Q}}\mathbf{P}\mathbf{I}\hat{\mathbf{U}} = \mathbf{I}\hat{\mathbf{Q}}\hat{\mathbf{U}}. \qquad (5.16)$$

(5.15) and (5.16) together imply that

$$\breve{w}(\mathbf{I}\hat{\mathbf{Q}}\hat{\mathbf{U}}, \mathbf{n}) = \breve{w}(\mathbf{I}\hat{\mathbf{U}}, \mathbf{n}) \quad \forall \mathbf{n} \in \mathrm{Unit}(\mathbb{E}^3), \quad \forall \hat{\mathbf{U}} \in \mathrm{Sym}^+(\mathbf{n}^\perp)$$

$$\forall \hat{\mathbf{Q}} \in \mathrm{Orth}_+(\mathbf{n}^\perp, \mathbf{n}^\perp). \qquad (5.17)$$

Equation (5.17) holds for all hyperelastic bodies, but material isotropy imposes the additional restricition that

$$\tilde{w}(\mathbf{FQ}, \mathbf{Q}^T \mathbf{n}) = \tilde{w}(\mathbf{F}, \mathbf{n}) \quad \forall \mathbf{F} \in \mathrm{Lin}_+(I\!\!E^3, I\!\!E^3), \quad \forall \mathbf{n} \in \mathrm{Unit}(I\!\!E^3),$$
$$\forall \mathbf{Q} \in \mathrm{Orth}_+(I\!\!E^3, I\!\!E^3). \tag{5.18}$$

Choose $\mathbf{Q} := \mathbf{I}\hat{\mathbf{Q}}\mathbf{P} + \mathbf{n} \otimes \mathbf{n}$, as in the previous claim, and note that

$$\mathbf{Q}^T \mathbf{n} = (\mathbf{I}\hat{\mathbf{Q}}^T \mathbf{P} + \mathbf{n} \otimes \mathbf{n})\mathbf{n} = \mathbf{n}.$$

Thus, isotropy implies that $\tilde{w}(\mathbf{FQ}, \mathbf{n}) = \tilde{w}(\mathbf{F}, \mathbf{n})$ for such a $\mathbf{Q}$ which, by the construction of $\check{w}$ in (4.7), gives that

$$\check{w}(\mathbf{FI}, \mathbf{n}) = \check{w}(\mathbf{FQI}, \mathbf{n}). \tag{5.19}$$

But

$$\mathbf{FQI} = \mathbf{F}(\mathbf{I}\hat{\mathbf{Q}}\mathbf{P} + \mathbf{n} \otimes \mathbf{n})\mathbf{I} = \mathbf{FI}\hat{\mathbf{Q}}\mathbf{PI} = \mathbf{FI}\hat{\mathbf{Q}}.$$

Equation (5.19) can thus be written as

$$\check{w}(I\!\!F, \mathbf{n}) = \check{w}(I\!\!F\hat{\mathbf{Q}}, \mathbf{n}), \tag{5.20}$$

and this holds for every $I\!\!F \in \mathrm{Lin}^{NS}(\mathbf{n}^\perp, I\!\!E^3)$, $\mathbf{n} \in \mathrm{Unit}(I\!\!E^3)$, $\hat{\mathbf{Q}} \in \mathrm{Orth}_+(\mathbf{n}^\perp, \mathbf{n}^\perp)$. Since $\mathbf{I}\hat{\mathbf{U}} \in \mathrm{Lin}^{NS}(\mathbf{n}^\perp, I\!\!E^3)$, (5.20) implies that

$$\check{w}(\mathbf{I}\hat{\mathbf{U}}, \mathbf{n}) = \check{w}(\mathbf{I}\hat{\mathbf{U}}\hat{\mathbf{Q}}, \mathbf{n}) \quad \forall \mathbf{n} \in \mathrm{Unit}(I\!\!E^3), \quad \forall \hat{\mathbf{U}} \in \mathrm{Sym}^+(\mathbf{n}^\perp),$$
$$\forall \hat{\mathbf{Q}} \in \mathrm{Orth}_+(\mathbf{n}^\perp, \mathbf{n}^\perp). \tag{5.21}$$

Equations (5.17) and (5.21) and the fact that the inclusion map $\mathbf{I}$ is determined solely by the unit normal $\mathbf{n}$ admits construction of an isotropic, scalar function

$$\bar{w}(\cdot, \mathbf{n}) : \mathrm{Sym}^+(\mathbf{n}^\perp) \to I\!\!R, \quad \forall \mathbf{n} \in \mathrm{Unit}(I\!\!E^3),$$

such that $\check{w}(\mathbf{I}\hat{\mathbf{U}}, \mathbf{n}) = \bar{w}(\hat{\mathbf{U}}, \mathbf{n}).$ $\qquad \square$

LEMMA 5. $\quad \partial_3 \hat{w}(i, j, \mathbf{n}) = 0 \quad \forall \{i, j, \mathbf{n}\} \in \hat{\mathcal{I}} \times \mathrm{Unit}(I\!\!E^3).$

Proof. Let $\mathbf{F}^* = \mathbf{FQ}$, $\mathbf{n}^* = \mathbf{Q}^T\mathbf{n}$, and $\mathbf{I}^* = \mathbf{Q}^T\mathbf{IQ}$, with $\mathbf{F} \in \text{Lin}_+(I\!E^3, I\!E^3)$, $\mathbf{n} \in \text{Unit}(I\!E^3)$, $\mathbf{Q} \in \text{Orth}_+(I\!E^3, I\!E^3)$, and $\mathbf{I}$ the inclusion map for $\mathbf{n}^\perp$. Let

$$\hat{\mathbf{U}}^* = \sqrt{(\mathbf{F}^*\mathbf{I}^*)^T(\mathbf{F}^*\mathbf{I}^*)}, \qquad \hat{\mathbf{U}} = \sqrt{(\mathbf{FI})^T(\mathbf{FI})}.$$

Then $\hat{\mathbf{U}}$ and $\hat{\mathbf{U}}^*$ have the same determinant since

$$j^2(\hat{\mathbf{U}}^*) = j\big(\mathbf{P}^*(\mathbf{F}^{*T}\mathbf{F}^*\mathbf{I}^*\big) = j(\mathbf{Q}^T\mathbf{PF}^T\mathbf{FIQ}) = j^2(\hat{\mathbf{U}}),$$

where both determinants must be positive. $\hat{\mathbf{U}}$ and $\hat{\mathbf{U}}^*$ must also have the same trace. This is true since

$$i(\hat{\mathbf{U}}^{*2}) = \big\langle \mathbf{P}^*\mathbf{F}^{*T}\mathbf{F}^*\mathbf{I}^*, 1_{\bar{s}} \big\rangle = \big\langle \mathbf{Q}^T\mathbf{PF}^T\mathbf{FIQ}, 1_{\bar{s}} \big\rangle$$
$$= \big\langle \mathbf{PF}^T\mathbf{FI}, 1_{\bar{s}} \big\rangle = i(\hat{\mathbf{U}}^2),$$

and

$$i(\hat{\mathbf{U}}) = \big[i(\hat{\mathbf{U}}^2) + 2j^2(\hat{\mathbf{U}})\big]^{1/2}.$$

Material isotropy implies that $\tilde{w}(\mathbf{F}, \mathbf{n}) = \tilde{w}(\mathbf{F}^*, \mathbf{n}^*)$, and in terms of $\hat{w}$ this means that

$$\hat{w}\big(i(\hat{\mathbf{U}}), j(\hat{\mathbf{U}}), \mathbf{n}\big) = \hat{w}\big(i(\hat{\mathbf{U}}^*), j(\hat{\mathbf{U}}^*), \mathbf{n}^*\big).$$

But $\hat{\mathbf{U}}$ and $\hat{\mathbf{U}}^*$ have the same trace and determinant so this equation is equivalent to

$$\hat{w}(i, j, \mathbf{n}) = \hat{w}(i, j, \mathbf{n}^*) \quad \forall \{i, j\} \in \hat{\mathcal{I}}, \quad \forall \mathbf{n}, \mathbf{n}^* \in \text{Unit}(I\!E^3). \qquad \square$$

Because of this result, the orientation dependence of $\hat{w}$ may be dropped and $\hat{w}$ considered a function $\hat{w} : \hat{\mathcal{I}} \to I\!R$.

By (4.23), a sufficient condition to guarantee isotropy for materials whose bulk is characterized by (5.2) is that

$$\tilde{w}(\mathbf{FQ}, \mathbf{Q}^T\mathbf{n}) = \tilde{w}(\mathbf{F}, \mathbf{n}) \quad \forall \mathbf{F} \in \text{Lin}_+(I\!E^3, I\!E^3), \quad \forall \mathbf{n} \in \text{Unit}(I\!E^3),$$
$$\forall \mathbf{Q} \in \text{Orth}_+(I\!E^3, I\!E^3).$$

In terms of $\hat{w}$ this is equivalent to

$$\hat{w}\big(i(\hat{\mathbf{U}}), j(\hat{\mathbf{U}})\big) = \hat{w}\big(i(\hat{\mathbf{U}}^*), j(\hat{\mathbf{U}}^*)\big) \quad \forall \mathbf{F} \in \text{Lin}_+(I\!E^3, I\!E^3), \quad \forall \mathbf{n} \in \text{Unit}(I\!E^3),$$
$$\forall \mathbf{Q} \in \text{Orth}_+(I\!E^3, I\!E^3),$$

where $\hat{U}$ and $\hat{U}^*$ are as defined in Lemma 5. But this equality is guaranteed since $\hat{U}$ and $\hat{U}^*$ have the same trace and determinant by Lemma 5. $\qquad\square$

The interface representation theorem is therefore established. In conjunction with its counterpart from the elasticity theory of bulk materials, this theorem implies that a necessary and sufficient condition for a hyperelastic material to be isotropic is that $(5.2)_1$ and (5.11) be satisfied. Note that the interfaces of such bodies are completely characterized b. two scalar invariants associated with the deformation of the interfaces *without regard* for interfacial orientation.

Equation $(4.17)_2$ gives the referential deformational surface stress $\hat{S}$ as a function of $\check{w}$ so the above result can be used to express $\hat{S}$ in terms of $\check{w}$. In the following discussion, a pr⸳ ⸳ ₊₍₎ndicates the directional derivative of a function. Also, it is convenient t⸳ ⵏ .roduce the two-dimensional right Cauchy-Green tensor $C_s := \hat{U}^2$. The directional derivative of $\check{w}$ with respect to its first argument is then given by

$$\langle \hat{S}, B \rangle = \check{w}'(F, \mathbf{n})B = \left[\partial_1\check{w}(i,j)i'(\hat{U}) + \partial_2\check{w}(i,j)j'(\hat{U})\right]\Phi'(C_s)\Gamma'(F)B \tag{5.22}$$
$$\forall B \in \mathrm{Lin}^{NS}(\mathbf{n}^\perp, E^3),$$

where

$$\Phi(C_s) := C_s^{1/2} \quad \forall C_s \in \mathrm{Sym}^+(\mathbf{n}^\perp)$$
$$\Gamma(F) := F^T F \quad \forall F \in \mathrm{Lin}^{NS}(\mathbf{n}^\perp, E^3). \tag{5.23}$$

A standard mathematical result (CIARLET [51] 10–11) is that

$$i'(\hat{U})\hat{D} = i(\hat{D}) \quad \forall \hat{U}, \hat{D} \in \mathrm{Sym}^+(\mathbf{n}^\perp)$$
$$j'(\hat{U})\hat{D} = j(\hat{U})i(\hat{U}^{-1}\hat{D}) \quad \forall \hat{U}, \hat{D} \in \mathrm{Sym}^+(\mathbf{n}^\perp). \tag{5.24}$$

Also,

$$\Gamma'(F)B = B^T F + F^T B \quad \forall F, B \in \mathrm{Lin}^{NS}(\mathbf{n}^\perp, E^3),$$
$$\Phi'(C_s)\hat{D} = \frac{1}{2}C_s^{-1/2}\hat{D} \quad C_s, \hat{D} \in \mathrm{Sym}^+(\mathbf{n}^\perp). \tag{5.25}$$

(5.25) implies that

$$\Phi'(C_s)[\Gamma'(F)B] = \frac{1}{2}\hat{U}^{-1}(B^T F + F^T B), \tag{5.26}$$

and this result can be used with $(5.24)_1$ to obtain

$$
\begin{aligned}
i'(\hat{\mathbf{U}})\Phi'(\mathbf{C}_s)\Gamma'(I\!\!F)I\!\!B &= \frac{1}{2}i\big[\hat{\mathbf{U}}^{-1}(I\!\!B^T I\!\!F + I\!\!F^T I\!\!B)\big] \\
&= \langle I\!\!F\hat{\mathbf{U}}^{-1}, I\!\!B\rangle.
\end{aligned}
\tag{5.27}
$$

Likewise, $(5.24)_2$ and (5.26) imply that

$$
\begin{aligned}
j'(\hat{\mathbf{U}})\Phi'(\mathbf{C}_s)\Gamma'(I\!\!F)I\!\!B &= \frac{1}{2}j(\hat{\mathbf{U}})\langle\hat{\mathbf{U}}^{-2}, I\!\!B^T I\!\!F + I\!\!F^T I\!\!B\rangle \\
&= j(\hat{\mathbf{U}})\langle I\!\!F\hat{\mathbf{U}}^{-2}, I\!\!B\rangle.
\end{aligned}
\tag{5.28}
$$

(5.27) and (5.28) can then be applied to (5.22) to obtain

$$
\begin{aligned}
\langle \hat{\mathbf{S}}, I\!\!B\rangle = {}&\partial_1\hat{w}(i,j)\langle I\!\!F\hat{\mathbf{U}}^{-1}, I\!\!B\rangle + \partial_2\hat{w}(i,j)j(\hat{\mathbf{U}})\langle I\!\!F\hat{\mathbf{U}}^{-2}, I\!\!B\rangle \\
&\forall\, I\!\!B \in \mathrm{Lin}^{NS}(\mathbf{n}^{\perp}, I\!\!E^3).
\end{aligned}
\tag{5.29}
$$

Therefore,

$$
\hat{\mathbf{S}} = \partial_1\hat{w}(i,j)I\!\!F\hat{\mathbf{U}}^{-1} + \partial_2\hat{w}(i,j)j(\hat{\mathbf{U}})I\!\!F\hat{\mathbf{U}}^{-2}
\tag{5.30}
$$

and

$$
\hat{\mathbf{T}} = \frac{1}{j}\partial_1\hat{w}(i,j)\bar{\mathbf{P}}I\!\!F\hat{\mathbf{U}}^{-1}\hat{\mathbf{F}}^T + \partial_2\hat{w}(i,j)\bar{\mathbf{P}}I\!\!F\hat{\mathbf{U}}^{-2}\hat{\mathbf{F}}^T.
\tag{5.31}
$$

These representations can be simplified by using the left polar decomposition of the surface deformation gradient. Given $\hat{\mathbf{F}} = \hat{\mathbf{Q}}\hat{\mathbf{U}} = \hat{\mathbf{V}}\hat{\mathbf{Q}}$, then $\hat{\mathbf{V}} = \hat{\mathbf{F}}\hat{\mathbf{U}}^{-1}\hat{\mathbf{F}}^T$. Therefore,

$$
\bar{\mathbf{P}}I\!\!F\hat{\mathbf{U}}^{-1}\hat{\mathbf{F}}^T = \hat{\mathbf{V}}.
\tag{5.32}
$$

A simplification is also possible by noting that

$$
\bar{\mathbf{P}}I\!\!F\hat{\mathbf{U}}^{-2}\hat{\mathbf{F}}^T = \mathbf{1}_{\bar{s}}.
\tag{5.33}
$$

Thus, the deformational stresses of isotropic, hyperelastic interfaces can be represented as

$$
\hat{\mathbf{S}} = \bar{\mathbf{I}}\big[\partial_1\hat{w}(i,j)\hat{\mathbf{F}}\hat{\mathbf{U}}^{-1} + j(\hat{\mathbf{U}})\partial_2\hat{w}(i,j)\hat{\mathbf{F}}^{-T}
\tag{5.34}
$$

and

$$
\hat{\mathbf{T}} = \frac{1}{j}\partial_1\hat{w}(i,j)\hat{\mathbf{V}} + \partial_2\hat{w}(i,j)\mathbf{1}_{\bar{s}}.
\tag{5.35}
$$

A representation for the accretive stress is then obtained using $(4.17)_3$.

6. Summary

A model for martensitic phase transitions has been presented that is intended to capture localized interfacial effects. A set of physically reasonable postulates lead to field equations and jump conditions. The notion of a hyperelastic material was extended to include bodies that support structured interfaces, and an interface representation theorem was derived for isotropic, hyperelastic bodies. The following is a summary of the interfacial characterization of these materials:

$$w = \hat{w}(i,j)$$
$$\hat{S} = \bar{I}\{(\partial_1\hat{w})\hat{F}\hat{U}^{-1} + (j\partial_2\hat{w})\hat{F}^{-T}\}$$
$$\hat{T} = \frac{1}{j}(\partial_1\hat{w})\hat{V} + (\partial_2\hat{w})\mathbf{1}_{\bar{s}}$$
$$\hat{C} = I\{-(\partial_1\hat{w})\hat{U} + (\hat{w} - j\partial_2\hat{w})\mathbf{1}_s\},$$

(6.1)

where

$$i := i(\hat{U}) = i(\hat{V}), \qquad j := j(\hat{U}) = j(\hat{V})$$
$$\hat{U} := \sqrt{\hat{F}^T\hat{F}}, \qquad \hat{V} := \sqrt{\hat{F}\hat{F}^T}.$$

Thus, isotropic, hyperelastic interfaces are completely characterized once the dependence of the surface energy on the invariants of the interfacial deformation is established. Moreover, a necessary and sufficient condition for a hyperelastic material to be isotropic is that $(5.2)_1$ and $(6.1)_1$ be satisfied.

An application of this theory is examined in LUSK [47], where three different interfacial constitutions are examined in a problem concerning nucleation and growth.

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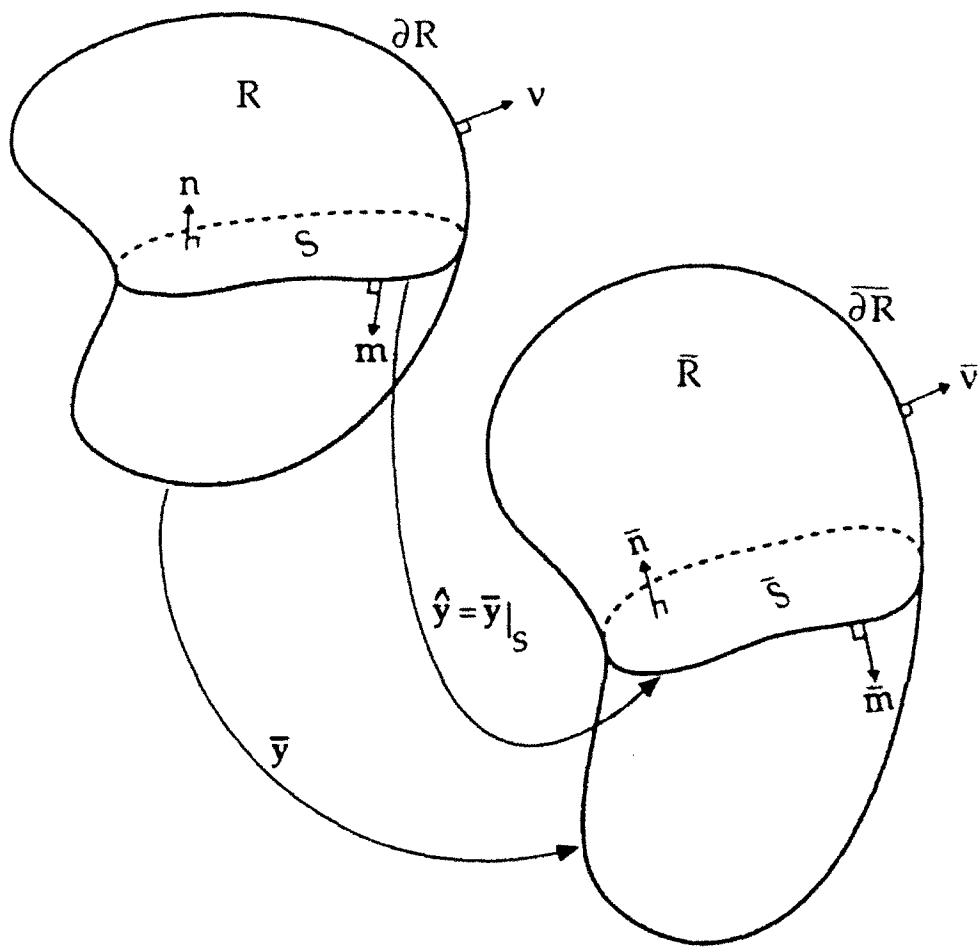
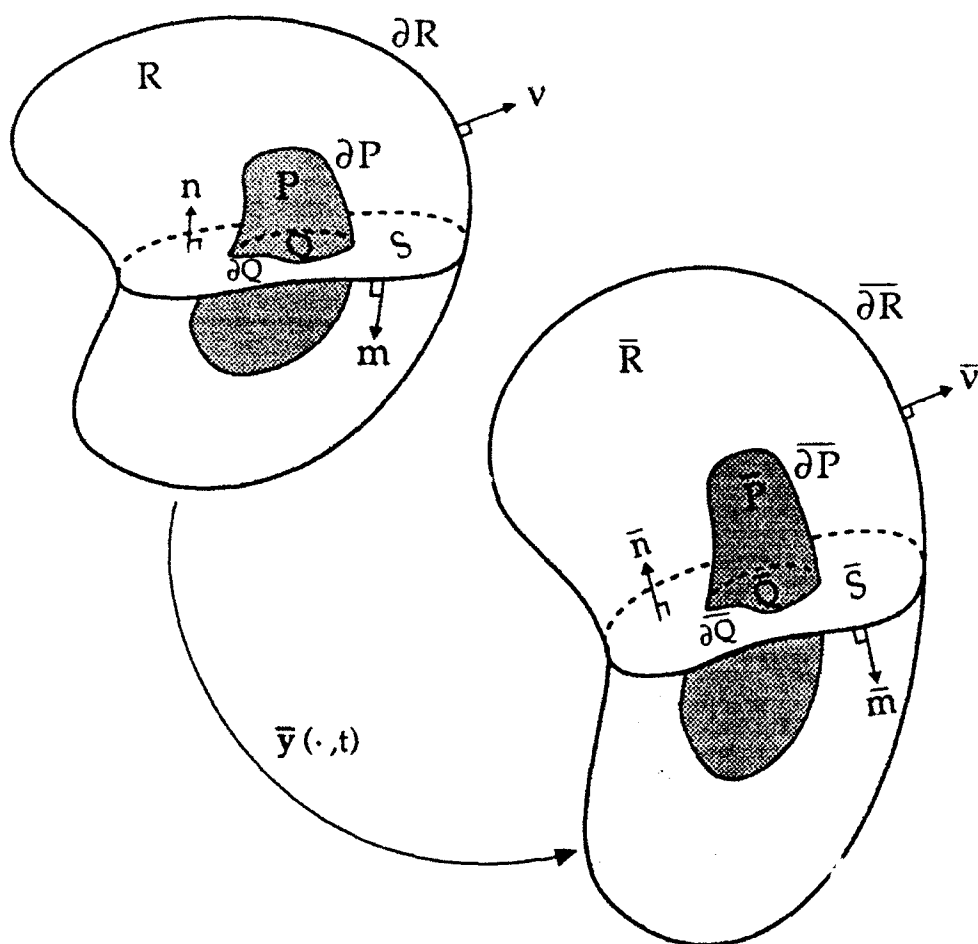Figure 1. A two-phase deformation $\bar{y}$ and its restriction $\hat{y}$ to the interface S.

Figure 2. Subregions P and Q(t) of R and S(t), respectively, and
their images $\bar{P}(t)$ and $\bar{Q}(t)$.

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ABSTRACT (Continue on reverse if necessary and identify by block number)
A model of martensitic phase transitions is presented that is capable of accounting
or a variety of surface effects associated with the localized interaction of coexisting
hases of a material. Such phenomena are thought to play a critical role in determining
he size, shape, and stability of nucleated embryos as well as to affect the conditions
nder which nucleation occurs. Attention is restricted to transitions that are mechanically
nduced, and the model does not account for temperature effects. Materials that undergo
artensitic phase changes are modeled as hyperelastic in both the bulk and the interface.
he characterization of such bodies is examined in detail, and a representation theorem
s presented for isotropic, hyperelastic interfaces in terms of two scalar invariants
ssociated with the deformation of the interface.

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